Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 01:43 AM EDT

PDB ID	:	3FVR
Title	:	Crystal Structure of Acetyl Xylan Esterase from Bacillus pumilus, monoclinic crystal form I
Authors	:	Krastanova, I.; Cassetta, A.; Lamba, D.
Deposited on	:	2009-01-16
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

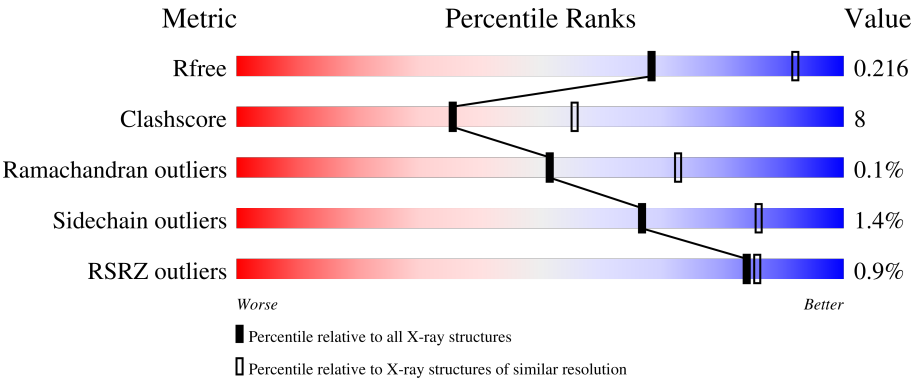
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	320	82% 17%
1	B	320	82% 17%
1	C	320	84% 16%
1	D	320	82% 17%
1	E	320	81% 18%

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Mol	Chain	Length	Quality of chain
1	F	320	84% 14%
1	G	320	83% 16%
1	H	320	81% 18%
1	I	320	81% 18%
1	L	320	80% 18%
1	M	320	81% 18%
1	N	320	80% 18%

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
4	PGE	C	323	-	-	X	-
5	PG4	H	322	-	-	X	-
6	PEG	M	321	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 32448 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2558	1659	419	476	4			
1	B	318	Total	C	N	O	S	0	0	0
			2544	1652	417	471	4			
1	C	320	Total	C	N	O	S	0	0	0
			2558	1659	419	476	4			
1	D	318	Total	C	N	O	S	0	0	0
			2544	1652	417	471	4			
1	E	318	Total	C	N	O	S	0	0	0
			2544	1652	417	471	4			
1	F	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	G	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	H	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	I	319	Total	C	N	O	S	0	0	0
			2550	1655	418	473	4			
1	L	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	M	318	Total	C	N	O	S	0	0	0
			2544	1652	417	471	4			
1	N	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	2	Total	Cl	0	0
			2	2		

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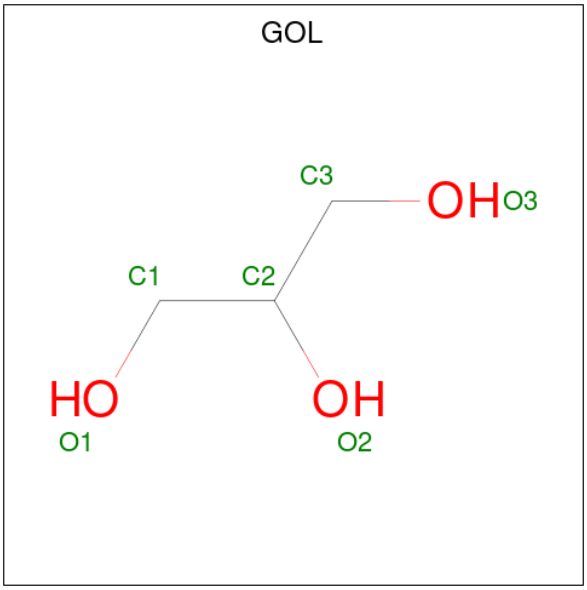
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Cl 2 2	0	0
2	D	2	Total Cl 2 2	0	0
2	E	2	Total Cl 2 2	0	0
2	F	2	Total Cl 2 2	0	0
2	G	2	Total Cl 2 2	0	0
2	H	2	Total Cl 2 2	0	0
2	I	2	Total Cl 2 2	0	0
2	L	2	Total Cl 2 2	0	0
2	M	2	Total Cl 2 2	0	0
2	N	2	Total Cl 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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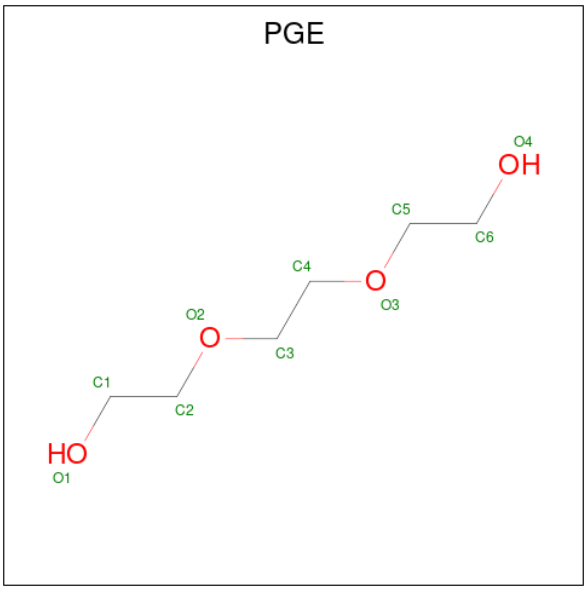
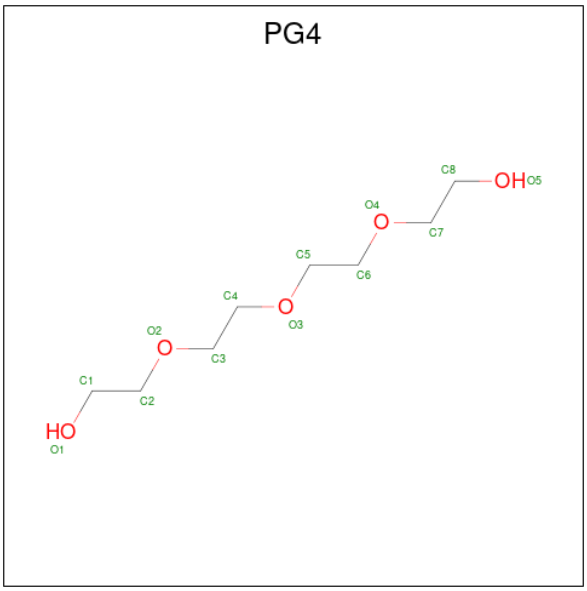
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



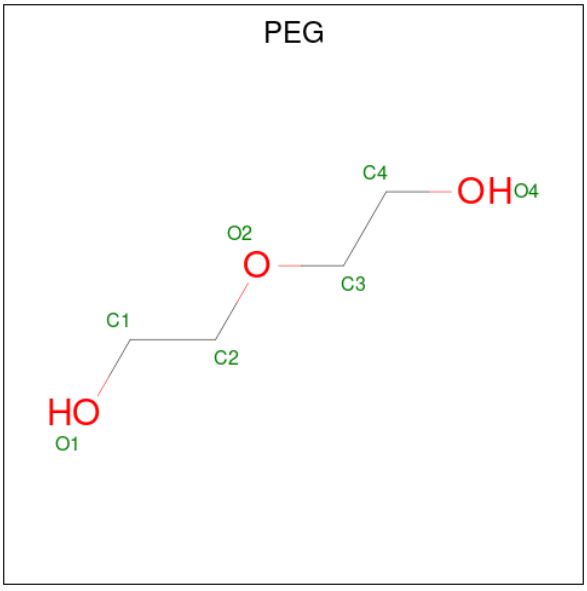
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 10 6 4	0	0
4	F	1	Total C O 10 6 4	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 13 8 5	0	0
5	G	1	Total C O 13 8 5	0	0
5	H	1	Total C O 13 8 5	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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

- Molecule 7 is water.

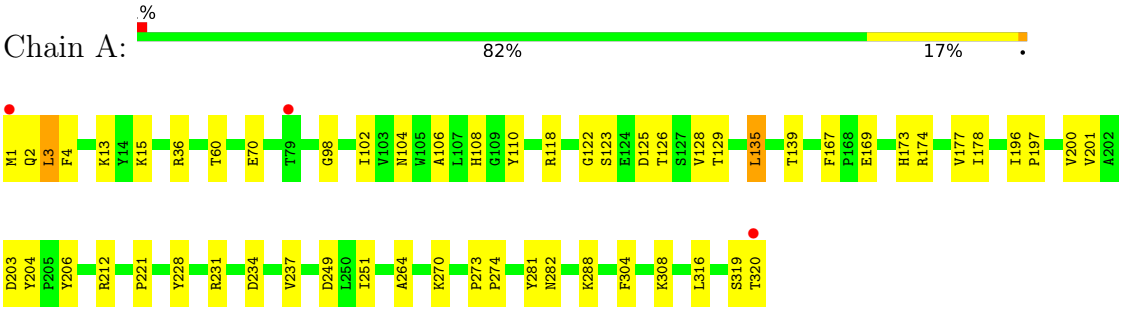
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	192	Total O 192 192	0	0
7	B	152	Total O 152 152	0	0
7	C	137	Total O 137 137	0	0
7	D	126	Total O 126 126	0	0
7	E	157	Total O 157 157	0	0
7	F	155	Total O 155 155	0	0
7	G	148	Total O 148 148	0	0
7	H	154	Total O 154 154	0	0
7	I	136	Total O 136 136	0	0
7	L	147	Total O 147 147	0	0
7	M	144	Total O 144 144	0	0
7	N	144	Total O 144 144	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.

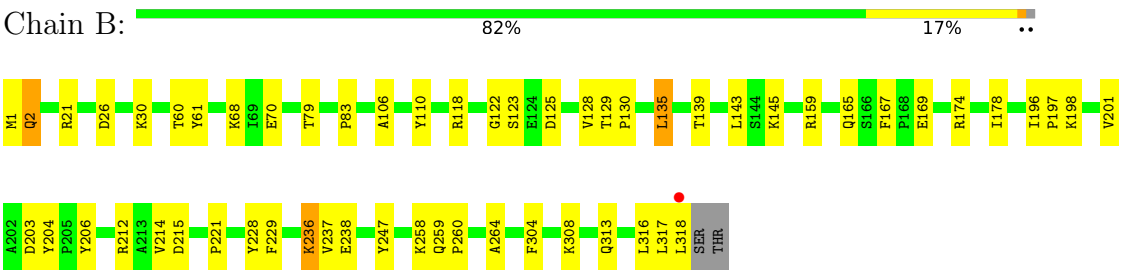
• Molecule 1: Acetyl xylan esterase

Chain A:



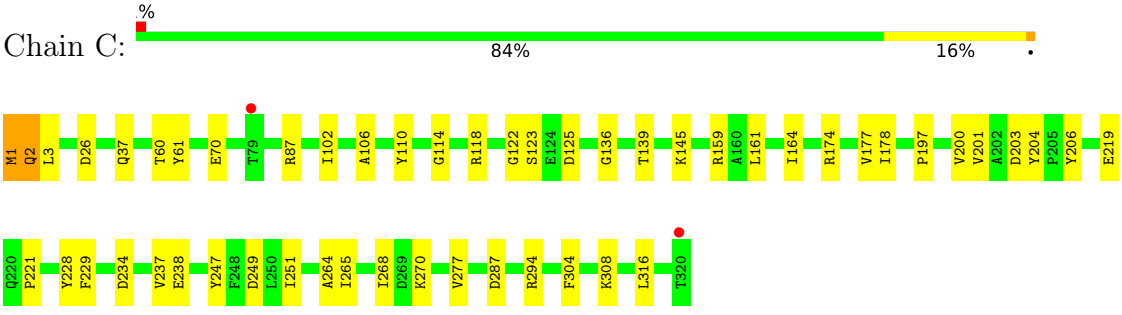
• Molecule 1: Acetyl xylan esterase

Chain B:



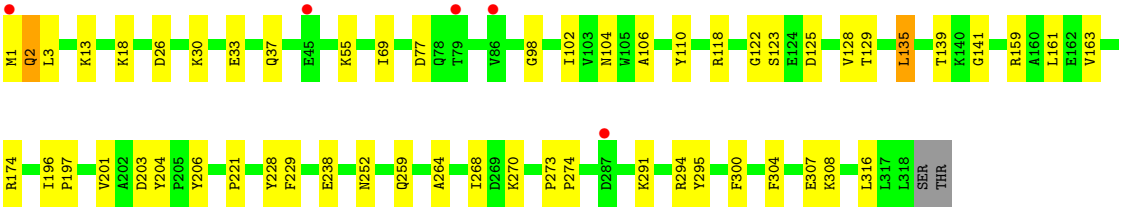
• Molecule 1: Acetyl xylan esterase

Chain C:

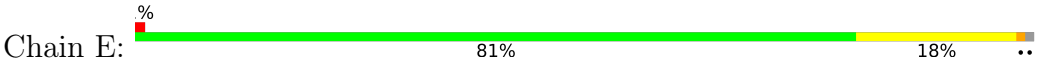


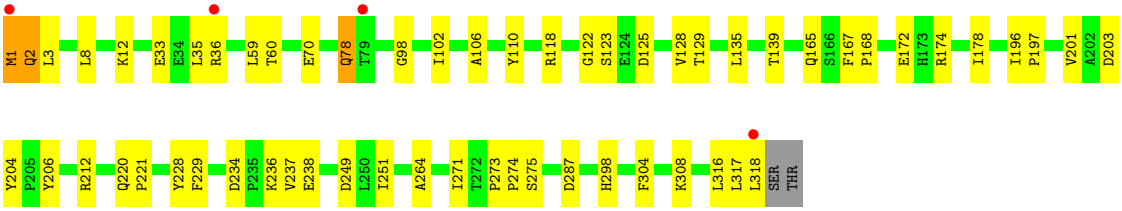
• Molecule 1: Acetyl xylan esterase

Chain D:

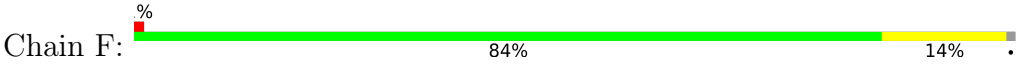


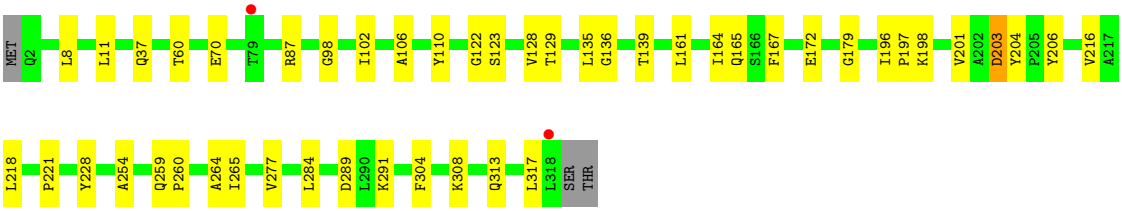
• Molecule 1: Acetyl xylan esterase



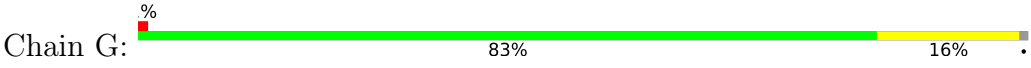


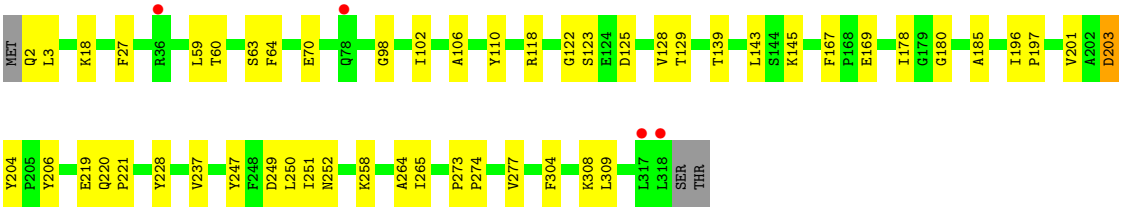
• Molecule 1: Acetyl xylan esterase



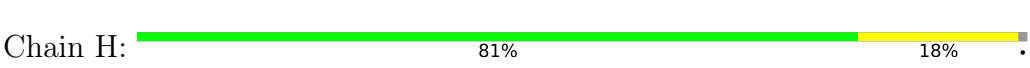


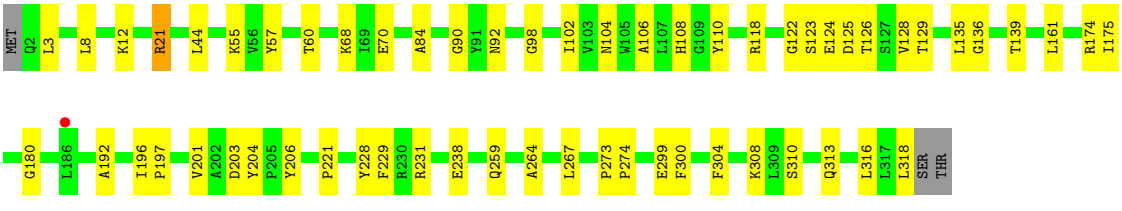
• Molecule 1: Acetyl xylan esterase





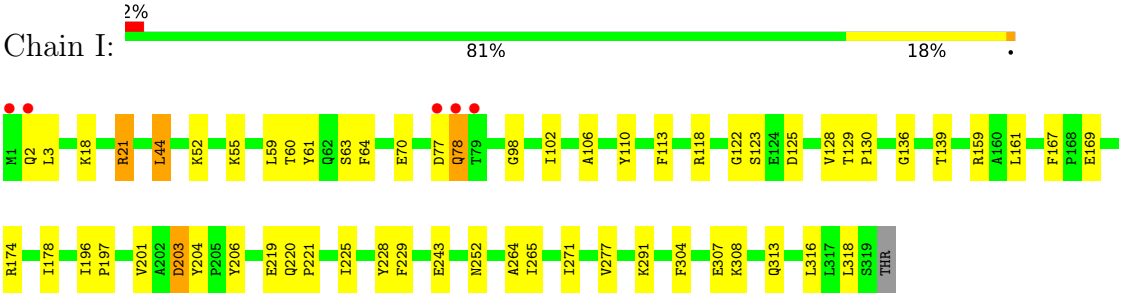
• Molecule 1: Acetyl xylan esterase





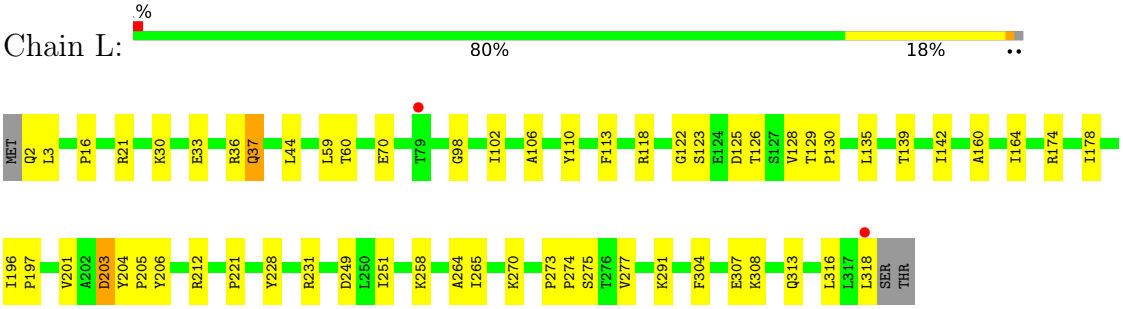
• Molecule 1: Acetyl xylan esterase

Chain I:



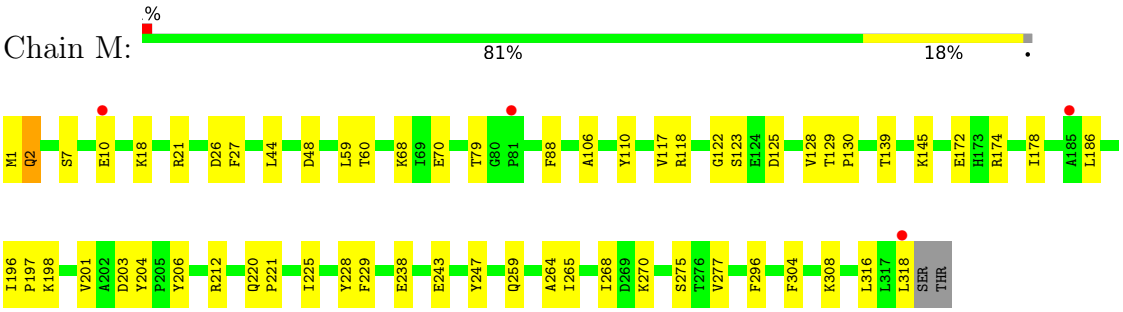
• Molecule 1: Acetyl xylan esterase

Chain L:



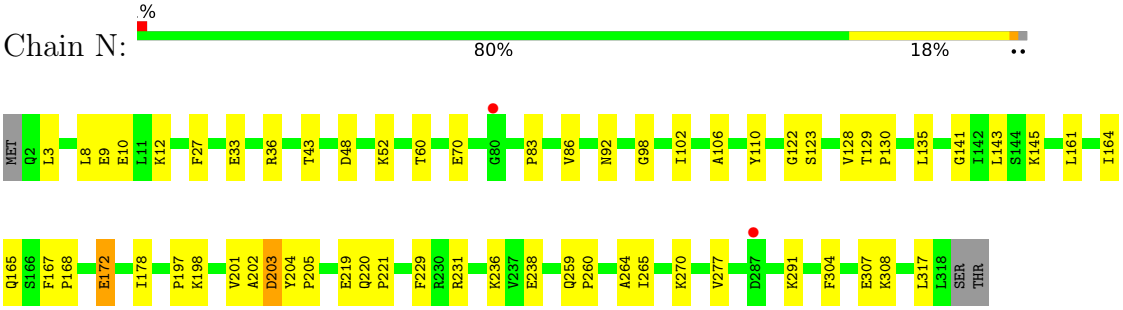
• Molecule 1: Acetyl xylan esterase

Chain M:



• Molecule 1: Acetyl xylan esterase

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.48Å 167.69Å 144.96Å 90.00° 91.35° 90.00°	Depositor
Resolution (Å)	29.90 – 2.50 29.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.90-2.50) 94.2 (29.93-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.184 , 0.228 0.172 , 0.216	Depositor DCC
R_{free} test set	13527 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	32448	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PGE, PG4, GOL, PEG

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	0.39	0/2630	0.60	0/3569
1	B	0.38	0/2616	0.59	0/3551
1	C	0.36	0/2630	0.59	0/3569
1	D	0.38	0/2616	0.59	0/3551
1	E	0.37	0/2616	0.59	0/3551
1	F	0.37	0/2608	0.58	0/3541
1	G	0.38	0/2608	0.58	0/3541
1	H	0.37	0/2608	0.59	0/3541
1	I	0.36	0/2622	0.58	0/3559
1	L	0.37	0/2608	0.59	0/3541
1	M	0.37	0/2616	0.59	0/3551
1	N	0.37	0/2608	0.58	0/3541
All	All	0.37	0/31386	0.59	0/42606

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	2558	0	2506	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2544	0	2494	41	0
1	C	2558	0	2506	44	0
1	D	2544	0	2494	48	0
1	E	2544	0	2494	41	0
1	F	2536	0	2482	36	0
1	G	2536	0	2482	32	0
1	H	2536	0	2482	49	0
1	I	2550	0	2499	42	0
1	L	2536	0	2482	42	0
1	M	2544	0	2494	50	0
1	N	2536	0	2482	41	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	1	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	1	0
3	C	12	0	16	1	0
3	F	6	0	8	0	0
3	I	6	0	8	0	0
3	L	6	0	8	0	0
4	C	10	0	14	9	0
4	F	10	0	14	2	0
5	D	13	0	18	0	0
5	G	13	0	18	1	0
5	H	13	0	18	8	0
6	H	14	0	20	2	0
6	M	7	0	10	6	0
7	A	192	0	0	3	0
7	B	152	0	0	5	0
7	C	137	0	0	2	0
7	D	126	0	0	2	0
7	E	157	0	0	3	0
7	F	155	0	0	3	0
7	G	148	0	0	1	0
7	H	154	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	136	0	0	0	0
7	L	147	0	0	2	0
7	M	144	0	0	4	0
7	N	144	0	0	3	0
All	All	32448	0	30049	494	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 8.

All (494) 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:D:1:MET:HG3	1:D:268:ILE:HD13	1.39	1.04
1:I:52:LYS:HD2	1:M:318:LEU:HD21	1.43	0.98
1:H:180:GLY:HA3	5:H:322:PG4:H52	1.46	0.93
1:B:60:THR:HG22	1:B:70:GLU:HG2	1.50	0.91
1:D:1:MET:HG2	1:D:2:GLN:N	1.86	0.91
1:G:60:THR:HG22	1:G:70:GLU:HG2	1.54	0.89
1:F:60:THR:HG22	1:F:70:GLU:HG2	1.53	0.88
1:D:1:MET:HG2	1:D:2:GLN:H	1.37	0.87
1:L:21:ARG:HG2	7:L:949:HOH:O	1.73	0.87
1:C:161:LEU:HD13	1:C:197:PRO:HD3	1.59	0.84
1:H:90:GLY:HA3	5:H:322:PG4:H71	1.60	0.83
5:H:322:PG4:H41	5:H:322:PG4:H12	1.60	0.81
1:C:60:THR:HG22	1:C:70:GLU:HG2	1.61	0.80
1:C:308:LYS:HD3	4:C:323:PGE:H62	1.62	0.80
1:B:313:GLN:HG2	1:B:318:LEU:HG	1.64	0.79
1:H:206:TYR:OH	1:H:221:PRO:HG2	1.83	0.79
1:H:60:THR:HG22	1:H:70:GLU:HG2	1.63	0.79
1:F:206:TYR:OH	1:F:221:PRO:HG2	1.81	0.79
1:G:206:TYR:OH	1:G:221:PRO:HG2	1.83	0.78
1:M:1:MET:SD	1:M:2:GLN:N	2.56	0.78
1:D:1:MET:HG3	1:D:268:ILE:CD1	2.13	0.78
1:M:201:VAL:HG11	1:M:308:LYS:HG3	1.67	0.77
1:M:60:THR:HG22	1:M:70:GLU:HG2	1.67	0.77
1:M:21:ARG:HD2	1:M:243:GLU:HG3	1.67	0.76
1:H:313:GLN:HG2	1:H:318:LEU:HG	1.68	0.76
1:H:300:PHE:HD1	5:H:322:PG4:H22	1.50	0.76
1:E:60:THR:HG22	1:E:70:GLU:HG2	1.67	0.76
1:D:1:MET:CG	1:D:2:GLN:H	1.92	0.76
1:B:201:VAL:HG11	1:B:308:LYS:HG3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:LEU:HD13	1:N:197:PRO:HD3	1.68	0.74
1:H:299:GLU:OE1	6:H:321:PEG:H41	1.87	0.73
1:A:1:MET:N	1:A:270:LYS:NZ	2.37	0.73
1:G:201:VAL:HG11	1:G:308:LYS:HG3	1.68	0.73
1:C:1:MET:N	1:C:270:LYS:HD3	2.04	0.73
1:I:206:TYR:OH	1:I:221:PRO:HG2	1.89	0.73
1:C:87:ARG:HG3	4:C:323:PGE:H3	1.71	0.73
1:A:60:THR:HG22	1:A:70:GLU:HG2	1.70	0.72
1:I:313:GLN:HG2	1:I:318:LEU:HG	1.72	0.71
1:I:60:THR:HG22	1:I:70:GLU:HG2	1.73	0.70
1:C:206:TYR:OH	1:C:221:PRO:HG2	1.91	0.70
1:B:206:TYR:OH	1:B:221:PRO:HG2	1.92	0.69
4:C:323:PGE:O2	4:C:323:PGE:H5	1.93	0.69
1:C:1:MET:SD	1:C:2:GLN:N	2.66	0.68
1:H:68:LYS:H	1:H:124:GLU:HG2	1.59	0.68
1:D:3:LEU:H	1:D:3:LEU:HD22	1.58	0.67
1:A:206:TYR:OH	1:A:221:PRO:HG2	1.94	0.67
1:D:26:ASP:O	1:D:30:LYS:HG2	1.95	0.67
1:D:206:TYR:OH	1:D:221:PRO:HG2	1.95	0.66
1:C:1:MET:HE2	1:C:2:GLN:H	1.60	0.66
1:M:221:PRO:HB3	6:M:321:PEG:H41	1.78	0.66
1:A:135:LEU:HD22	1:F:135:LEU:CD2	2.24	0.66
1:H:161:LEU:HD13	1:H:197:PRO:HD3	1.76	0.66
1:F:179:GLY:HA2	4:F:322:PGE:H2	1.75	0.66
1:C:178:ILE:HB	4:C:323:PGE:H6	1.78	0.66
1:E:206:TYR:OH	1:E:221:PRO:HG2	1.94	0.66
1:M:265:ILE:HD13	1:M:277:VAL:HG21	1.78	0.66
1:M:206:TYR:OH	1:M:221:PRO:HG2	1.97	0.65
1:I:52:LYS:HD2	1:M:318:LEU:CD2	2.23	0.65
1:A:319:SER:HB2	7:A:736:HOH:O	1.96	0.65
1:G:206:TYR:CZ	1:G:221:PRO:HG2	2.32	0.65
1:G:309:LEU:HD11	5:G:321:PG4:H81	1.78	0.65
1:D:2:GLN:OE1	1:D:2:GLN:HA	1.95	0.64
1:D:174:ARG:HD2	1:D:316:LEU:O	1.96	0.64
3:C:322:GOL:H32	1:D:104:ASN:HD21	1.62	0.64
1:B:258:LYS:HE2	7:B:797:HOH:O	1.97	0.64
1:D:291:LYS:HE3	1:D:307:GLU:OE1	1.98	0.64
1:E:318:LEU:HB2	7:E:1409:HOH:O	1.96	0.64
1:B:206:TYR:CZ	1:B:221:PRO:HG2	2.34	0.63
1:F:265:ILE:HD13	1:F:277:VAL:HG21	1.80	0.63
1:H:264:ALA:HB2	1:H:304:PHE:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:VAL:HG11	1:I:308:LYS:HG3	1.81	0.62
1:L:313:GLN:HG2	1:L:318:LEU:HG	1.81	0.62
1:H:206:TYR:CZ	1:H:221:PRO:HG2	2.35	0.62
1:F:206:TYR:CZ	1:F:221:PRO:HG2	2.35	0.61
1:C:234:ASP:HB3	1:C:237:VAL:HG23	1.82	0.61
1:A:178:ILE:HG22	1:A:201:VAL:HB	1.83	0.61
1:C:206:TYR:CZ	1:C:221:PRO:HG2	2.35	0.61
1:L:36:ARG:HG2	1:L:36:ARG:HH11	1.65	0.61
1:M:59:LEU:HD12	1:M:60:THR:N	2.15	0.61
1:H:300:PHE:CD1	5:H:322:PG4:H22	2.35	0.61
1:D:1:MET:O	1:D:270:LYS:NZ	2.34	0.61
1:C:201:VAL:HG11	1:C:308:LYS:HG3	1.81	0.61
1:H:201:VAL:HG11	1:H:308:LYS:HG3	1.81	0.60
1:L:206:TYR:OH	1:L:221:PRO:HG2	2.01	0.60
1:C:3:LEU:HD21	1:C:294:ARG:CZ	2.31	0.60
1:A:201:VAL:HG11	1:A:308:LYS:HG3	1.83	0.60
1:N:165:GLN:HG3	1:N:172:GLU:HB3	1.84	0.60
1:E:33:GLU:HA	1:E:36:ARG:HG2	1.83	0.59
1:C:136:GLY:HA2	1:E:135:LEU:HD11	1.84	0.59
1:L:178:ILE:HG22	1:L:201:VAL:HB	1.84	0.59
1:A:206:TYR:CZ	1:A:221:PRO:HG2	2.38	0.58
1:A:1:MET:H2	1:A:270:LYS:NZ	2.00	0.58
1:C:136:GLY:HA2	1:E:135:LEU:CD1	2.32	0.58
1:M:220:GLN:HG3	6:M:321:PEG:H32	1.84	0.58
1:C:3:LEU:HD22	1:C:3:LEU:H	1.68	0.58
1:D:206:TYR:CZ	1:D:221:PRO:HG2	2.39	0.58
1:E:206:TYR:CZ	1:E:221:PRO:HG2	2.38	0.58
1:M:220:GLN:HB2	6:M:321:PEG:H21	1.84	0.58
1:L:196:ILE:HB	1:L:197:PRO:HD3	1.85	0.58
1:M:1:MET:N	1:M:270:LYS:NZ	2.51	0.58
1:B:167:PHE:HB3	1:B:169:GLU:OE1	2.04	0.57
1:B:264:ALA:HB2	1:B:304:PHE:CE1	2.38	0.57
1:E:201:VAL:HG11	1:E:308:LYS:HG3	1.86	0.57
1:C:1:MET:CE	1:C:2:GLN:H	2.17	0.57
1:B:143:LEU:HD21	1:B:237:VAL:HG13	1.87	0.57
1:M:221:PRO:HB3	6:M:321:PEG:H22	1.87	0.57
1:L:2:GLN:N	1:L:270:LYS:HZ1	2.03	0.57
1:C:264:ALA:HB2	1:C:304:PHE:CE1	2.39	0.56
1:F:179:GLY:CA	4:F:322:PGE:H2	2.35	0.56
1:M:18:LYS:NZ	7:M:738:HOH:O	2.38	0.56
1:A:319:SER:O	1:A:320:THR:HB	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ASP:OD1	1:E:251:ILE:HG12	2.05	0.56
1:N:201:VAL:HG11	1:N:308:LYS:HG3	1.86	0.56
1:C:61:TYR:CE2	1:C:159:ARG:HG3	2.41	0.56
1:D:201:VAL:HG11	1:D:308:LYS:HG3	1.88	0.56
1:B:83:PRO:HG3	1:B:317:LEU:HD12	1.88	0.55
1:M:27:PHE:CD1	1:M:145:LYS:HD2	2.42	0.55
1:M:220:GLN:CB	6:M:321:PEG:H32	2.36	0.55
1:E:1:MET:O	1:E:2:GLN:O	2.25	0.55
1:M:1:MET:H2	1:M:270:LYS:NZ	2.05	0.55
1:N:202:ALA:HB1	1:N:205:PRO:HG3	1.88	0.54
1:C:1:MET:H1	1:C:270:LYS:HD3	1.73	0.54
1:H:92:ASN:ND2	7:H:462:HOH:O	2.36	0.54
1:N:43:THR:HG1	1:N:60:THR:HG1	1.54	0.54
1:I:206:TYR:CZ	1:I:221:PRO:HG2	2.42	0.54
1:C:87:ARG:HE	4:C:323:PGE:C3	2.20	0.54
1:E:122:GLY:O	1:E:123:SER:HB2	2.07	0.54
1:B:178:ILE:HG22	1:B:201:VAL:HB	1.90	0.54
1:M:172:GLU:HG2	7:M:345:HOH:O	2.07	0.54
1:G:196:ILE:HB	1:G:197:PRO:HD3	1.89	0.54
1:L:291:LYS:HE3	1:L:307:GLU:OE1	2.08	0.54
1:E:172:GLU:HG3	7:E:1410:HOH:O	2.08	0.53
1:E:178:ILE:HG22	1:E:201:VAL:HB	1.90	0.53
1:H:68:LYS:H	1:H:124:GLU:CG	2.21	0.53
1:H:8:LEU:HG	1:H:12:LYS:HE3	1.91	0.53
1:M:1:MET:H2	1:M:270:LYS:HZ3	1.56	0.53
1:I:174:ARG:HD2	1:I:316:LEU:O	2.08	0.53
1:A:174:ARG:HD3	1:A:320:THR:OG1	2.09	0.53
1:D:3:LEU:HD21	1:D:294:ARG:CZ	2.39	0.53
1:C:219:GLU:HB3	7:C:1332:HOH:O	2.08	0.53
1:F:264:ALA:HB2	1:F:304:PHE:CE1	2.44	0.53
1:N:264:ALA:HB2	1:N:304:PHE:CE1	2.43	0.53
1:C:87:ARG:NE	4:C:323:PGE:H32	2.23	0.53
1:D:18:LYS:HE3	1:D:252:ASN:HA	1.91	0.53
1:H:128:VAL:HG12	1:H:129:THR:N	2.24	0.53
1:I:18:LYS:HE3	1:I:252:ASN:HA	1.91	0.53
1:I:59:LEU:HD12	1:I:60:THR:N	2.24	0.53
1:D:161:LEU:HD13	1:D:197:PRO:HD3	1.90	0.52
1:H:21:ARG:NH1	1:H:21:ARG:HG3	2.25	0.52
1:G:59:LEU:HD12	1:G:60:THR:N	2.24	0.52
1:H:98:GLY:O	1:H:102:ILE:HG12	2.07	0.52
1:C:87:ARG:NE	4:C:323:PGE:C3	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:236:LYS:HD3	7:N:643:HOH:O	2.08	0.52
1:F:317:LEU:HD21	7:F:735:HOH:O	2.09	0.52
1:I:122:GLY:O	1:I:123:SER:HB2	2.09	0.52
1:M:59:LEU:HD12	1:M:60:THR:H	1.74	0.52
1:F:135:LEU:C	1:F:135:LEU:HD23	2.29	0.52
1:E:8:LEU:O	1:E:12:LYS:HG3	2.09	0.52
1:E:234:ASP:HB3	1:E:237:VAL:HG23	1.92	0.52
1:I:61:TYR:CE2	1:I:159:ARG:HG3	2.45	0.52
1:B:174:ARG:HD2	1:B:316:LEU:O	2.09	0.52
1:D:300:PHE:HA	7:D:1631:HOH:O	2.10	0.52
1:G:264:ALA:HB2	1:G:304:PHE:CE1	2.45	0.51
1:I:265:ILE:HD13	1:I:277:VAL:HG21	1.90	0.51
1:A:135:LEU:CD2	1:F:136:GLY:HA2	2.40	0.51
1:L:60:THR:HG22	1:L:70:GLU:HG2	1.92	0.51
1:M:44:LEU:CD1	1:M:59:LEU:HD13	2.40	0.51
1:H:128:VAL:HG13	1:L:126:THR:HA	1.92	0.51
1:I:220:GLN:O	1:I:271:ILE:HG23	2.10	0.51
1:I:264:ALA:HB2	1:I:304:PHE:CE1	2.45	0.51
1:C:249:ASP:OD1	1:C:251:ILE:HG12	2.11	0.51
1:M:128:VAL:O	1:M:130:PRO:HD3	2.10	0.51
1:E:1:MET:SD	1:E:1:MET:N	2.75	0.51
1:D:196:ILE:N	1:D:197:PRO:HD2	2.25	0.51
1:D:264:ALA:HB2	1:D:304:PHE:CE1	2.46	0.51
1:H:180:GLY:HA3	5:H:322:PG4:H42	1.92	0.51
1:L:206:TYR:CZ	1:L:221:PRO:HG2	2.46	0.51
5:H:322:PG4:H41	5:H:322:PG4:C1	2.34	0.51
1:L:249:ASP:OD1	1:L:251:ILE:HG12	2.10	0.51
1:B:135:LEU:HD22	1:D:135:LEU:HD22	1.91	0.50
1:H:180:GLY:CA	5:H:322:PG4:H52	2.31	0.50
1:L:118:ARG:HB3	1:L:125:ASP:HB2	1.93	0.50
1:N:27:PHE:CD1	1:N:145:LYS:HD2	2.46	0.50
1:B:122:GLY:O	1:B:123:SER:HB2	2.11	0.50
1:I:55:LYS:HE2	1:I:77:ASP:OD2	2.11	0.50
1:L:30:LYS:HB2	1:L:30:LYS:NZ	2.27	0.50
1:N:8:LEU:HG	1:N:12:LYS:NZ	2.26	0.50
1:I:59:LEU:HD23	1:I:113:PHE:CD1	2.47	0.50
1:N:83:PRO:HG3	1:N:317:LEU:HD12	1.94	0.50
1:N:265:ILE:HD13	1:N:277:VAL:HG21	1.94	0.50
1:M:264:ALA:HB2	1:M:304:PHE:CE1	2.46	0.50
1:D:197:PRO:HG2	1:D:259:GLN:NE2	2.27	0.50
1:E:236:LYS:HD2	7:E:1660:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:59:LEU:HD12	1:L:60:THR:N	2.26	0.50
1:G:2:GLN:N	7:G:327:HOH:O	2.45	0.50
1:G:178:ILE:HG22	1:G:201:VAL:HB	1.94	0.50
1:I:52:LYS:CD	1:M:318:LEU:HD21	2.30	0.50
1:H:264:ALA:HB2	1:H:304:PHE:CD1	2.47	0.49
1:N:9:GLU:HG2	1:N:10:GLU:N	2.26	0.49
1:G:249:ASP:OD1	1:G:251:ILE:HG12	2.12	0.49
1:H:68:LYS:N	1:H:124:GLU:HG2	2.25	0.49
1:C:122:GLY:O	1:C:123:SER:HB2	2.12	0.49
1:G:139:THR:HG21	1:G:228:TYR:HB2	1.94	0.49
1:M:106:ALA:HA	1:M:110:TYR:O	2.11	0.49
1:A:118:ARG:HB3	1:A:125:ASP:HB2	1.95	0.49
1:H:104:ASN:O	1:H:108:HIS:HD2	1.95	0.49
1:G:185:ALA:HA	1:G:250:LEU:HD11	1.94	0.49
1:N:122:GLY:O	1:N:123:SER:HB2	2.11	0.49
1:A:135:LEU:HD22	1:F:135:LEU:HD21	1.92	0.49
1:D:106:ALA:HA	1:D:110:TYR:O	2.12	0.49
1:G:180:GLY:HA2	1:G:203:ASP:HB2	1.94	0.49
1:M:196:ILE:N	1:M:197:PRO:HD2	2.28	0.49
1:C:308:LYS:CD	4:C:323:PGE:H62	2.39	0.49
1:L:106:ALA:HA	1:L:110:TYR:O	2.13	0.49
1:D:229:PHE:CE1	1:D:238:GLU:HA	2.48	0.48
1:H:180:GLY:HA2	1:H:203:ASP:HB2	1.94	0.48
1:L:33:GLU:OE2	1:L:37:GLN:NE2	2.46	0.48
1:L:139:THR:HG21	1:L:228:TYR:HB2	1.95	0.48
1:A:106:ALA:HA	1:A:110:TYR:O	2.14	0.48
1:N:205:PRO:HD2	1:N:277:VAL:HG13	1.94	0.48
1:A:1:MET:H3	1:A:270:LYS:NZ	2.09	0.48
1:D:3:LEU:HD21	1:D:294:ARG:NH2	2.28	0.48
1:G:122:GLY:O	1:G:123:SER:HB2	2.14	0.48
1:F:106:ALA:HA	1:F:110:TYR:O	2.13	0.48
1:A:122:GLY:O	1:A:123:SER:HB2	2.14	0.48
1:E:59:LEU:HD12	1:E:60:THR:H	1.79	0.48
1:H:106:ALA:HA	1:H:110:TYR:O	2.14	0.48
1:H:118:ARG:HB3	1:H:125:ASP:HB2	1.95	0.48
1:M:1:MET:O	1:M:270:LYS:NZ	2.46	0.48
1:A:264:ALA:HB2	1:A:304:PHE:CE1	2.49	0.48
1:M:139:THR:HG21	1:M:228:TYR:HB2	1.96	0.48
1:A:98:GLY:O	1:A:102:ILE:HG12	2.14	0.47
1:B:61:TYR:CE2	1:B:159:ARG:HG3	2.49	0.47
1:E:118:ARG:HB3	1:E:125:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:HG2	7:B:1059:HOH:O	2.14	0.47
1:E:8:LEU:HG	1:E:12:LYS:HE3	1.96	0.47
1:E:212:ARG:HE	1:E:275:SER:CB	2.26	0.47
1:E:317:LEU:O	1:E:318:LEU:HB2	2.14	0.47
1:M:122:GLY:O	1:M:123:SER:HB2	2.14	0.47
1:M:178:ILE:HG22	1:M:201:VAL:HB	1.95	0.47
1:N:8:LEU:HG	1:N:12:LYS:HZ3	1.79	0.47
1:C:61:TYR:CD2	1:C:159:ARG:HG3	2.49	0.47
1:D:1:MET:HG2	1:D:268:ILE:HG21	1.96	0.47
1:D:55:LYS:HE2	1:D:77:ASP:HA	1.97	0.47
1:D:69:ILE:N	1:D:69:ILE:HD12	2.29	0.47
1:F:122:GLY:O	1:F:123:SER:HB2	2.15	0.47
1:A:1:MET:HB2	7:C:1625:HOH:O	2.14	0.47
1:A:177:VAL:CG2	1:A:200:VAL:HG22	2.44	0.47
1:B:214:VAL:HG23	1:B:215:ASP:OD1	2.15	0.47
1:C:106:ALA:HA	1:C:110:TYR:O	2.14	0.47
1:D:159:ARG:O	1:D:163:VAL:HG23	2.15	0.47
1:I:106:ALA:HA	1:I:110:TYR:O	2.14	0.47
1:M:206:TYR:CZ	1:M:221:PRO:HG2	2.49	0.47
1:D:1:MET:HE1	1:D:295:TYR:HD1	1.80	0.47
1:D:139:THR:HG21	1:D:228:TYR:HB2	1.96	0.47
1:E:264:ALA:HB2	1:E:304:PHE:CE1	2.50	0.47
1:I:161:LEU:HD13	1:I:197:PRO:HG3	1.96	0.47
1:N:106:ALA:HA	1:N:110:TYR:O	2.14	0.47
1:C:1:MET:H2	1:C:270:LYS:HD3	1.79	0.47
1:C:145:LYS:HD3	1:C:247:TYR:CE2	2.50	0.47
1:E:128:VAL:HG12	1:E:129:THR:N	2.30	0.47
1:G:167:PHE:HB3	1:G:169:GLU:OE1	2.14	0.47
1:L:36:ARG:HG2	1:L:36:ARG:NH1	2.29	0.47
1:G:106:ALA:HA	1:G:110:TYR:O	2.16	0.46
1:H:21:ARG:HH11	1:H:21:ARG:CG	2.28	0.46
1:B:60:THR:CG2	1:B:70:GLU:HG2	2.33	0.46
1:H:174:ARG:HD2	1:H:316:LEU:O	2.16	0.46
1:N:86:VAL:HG21	1:N:161:LEU:HD23	1.97	0.46
1:D:1:MET:CG	1:D:268:ILE:HG21	2.45	0.46
1:F:60:THR:CG2	1:F:70:GLU:HG2	2.34	0.46
1:L:122:GLY:O	1:L:123:SER:HB2	2.16	0.46
1:A:203:ASP:O	1:A:204:TYR:C	2.54	0.46
1:B:106:ALA:HA	1:B:110:TYR:O	2.15	0.46
1:A:234:ASP:HB3	1:A:237:VAL:HG23	1.96	0.46
1:G:27:PHE:CD1	1:G:145:LYS:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:GLY:O	1:I:102:ILE:HG12	2.15	0.46
1:I:128:VAL:O	1:I:130:PRO:HD3	2.15	0.46
1:M:68:LYS:HD2	7:M:747:HOH:O	2.16	0.46
1:N:270:LYS:HB2	1:N:270:LYS:NZ	2.30	0.46
1:A:15:LYS:HE2	1:A:282:ASN:O	2.15	0.46
1:C:229:PHE:CE1	1:C:238:GLU:HA	2.51	0.46
1:E:59:LEU:HD12	1:E:60:THR:N	2.31	0.46
1:F:98:GLY:O	1:F:102:ILE:HG12	2.16	0.46
1:I:61:TYR:CD2	1:I:159:ARG:HG3	2.51	0.46
1:L:98:GLY:O	1:L:102:ILE:HG12	2.16	0.46
1:L:212:ARG:HE	1:L:275:SER:CB	2.28	0.46
1:L:264:ALA:HB2	1:L:304:PHE:CE1	2.51	0.46
1:B:2:GLN:OE1	1:B:2:GLN:HA	2.16	0.46
1:E:106:ALA:HA	1:E:110:TYR:O	2.15	0.46
1:M:220:GLN:CG	6:M:321:PEG:H32	2.46	0.46
1:G:145:LYS:HD3	1:G:247:TYR:CE2	2.50	0.46
1:I:203:ASP:O	1:I:204:TYR:C	2.54	0.46
1:L:174:ARG:HD2	1:L:316:LEU:O	2.16	0.46
1:M:174:ARG:HD2	1:M:316:LEU:O	2.16	0.46
1:N:164:ILE:HD13	1:N:167:PHE:CE2	2.51	0.46
1:A:174:ARG:HD2	1:A:316:LEU:O	2.15	0.46
1:L:128:VAL:O	1:L:130:PRO:HD3	2.16	0.46
1:B:135:LEU:HD22	1:D:135:LEU:CD2	2.46	0.45
1:B:203:ASP:O	1:B:204:TYR:C	2.54	0.45
1:G:273:PRO:HA	1:G:274:PRO:HD3	1.90	0.45
1:C:203:ASP:O	1:C:204:TYR:C	2.55	0.45
1:C:1:MET:HE2	1:C:268:ILE:HG21	1.97	0.45
1:G:128:VAL:HG12	1:G:129:THR:N	2.31	0.45
1:A:196:ILE:N	1:A:197:PRO:HD2	2.31	0.45
1:D:128:VAL:HG12	1:D:129:THR:N	2.30	0.45
1:H:21:ARG:NH2	7:H:1592:HOH:O	2.49	0.45
1:H:203:ASP:O	1:H:204:TYR:C	2.53	0.45
1:M:203:ASP:O	1:M:204:TYR:C	2.54	0.45
1:B:229:PHE:CE1	1:B:238:GLU:HA	2.51	0.45
1:B:264:ALA:HB2	1:B:304:PHE:CZ	2.51	0.45
1:H:231:ARG:HG3	1:H:231:ARG:HH11	1.82	0.45
1:I:178:ILE:HG22	1:I:201:VAL:HB	1.98	0.45
1:D:118:ARG:HB3	1:D:125:ASP:HB2	1.99	0.45
1:H:135:LEU:CD2	1:L:135:LEU:HD22	2.47	0.45
1:E:196:ILE:HB	1:E:197:PRO:HD3	1.99	0.45
1:L:128:VAL:HG12	1:L:129:THR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:HB3	7:B:346:HOH:O	2.17	0.45
1:D:33:GLU:O	1:D:37:GLN:HG3	2.17	0.45
1:E:78:GLN:HE21	1:E:78:GLN:HB3	1.53	0.45
1:F:139:THR:HG21	1:F:228:TYR:HB2	1.99	0.45
1:G:203:ASP:O	1:G:204:TYR:C	2.55	0.45
1:L:59:LEU:HD12	1:L:60:THR:H	1.82	0.45
1:L:231:ARG:HG3	1:L:231:ARG:HH11	1.81	0.45
1:F:216:VAL:O	1:F:218:LEU:HD22	2.17	0.45
1:I:225:ILE:HG22	1:I:229:PHE:CE2	2.52	0.45
1:A:231:ARG:HG3	1:A:231:ARG:HH11	1.81	0.45
1:I:139:THR:HG21	1:I:228:TYR:HB2	1.99	0.45
1:I:291:LYS:HE3	1:I:307:GLU:OE1	2.17	0.45
1:E:203:ASP:O	1:E:204:TYR:C	2.55	0.44
1:G:59:LEU:HD12	1:G:60:THR:H	1.81	0.44
1:G:118:ARG:HB3	1:G:125:ASP:HB2	1.99	0.44
1:I:196:ILE:N	1:I:197:PRO:CD	2.80	0.44
1:N:229:PHE:CE1	1:N:238:GLU:HA	2.52	0.44
1:A:1:MET:H2	1:A:270:LYS:HZ2	1.64	0.44
1:D:273:PRO:HA	1:D:274:PRO:HD3	1.95	0.44
1:F:128:VAL:HG12	1:F:129:THR:N	2.32	0.44
1:M:229:PHE:CE1	1:M:238:GLU:HA	2.53	0.44
1:N:264:ALA:HB2	1:N:304:PHE:CD1	2.53	0.44
1:A:104:ASN:O	1:A:108:HIS:HD2	2.00	0.44
1:C:270:LYS:HE3	1:C:270:LYS:HB2	1.79	0.44
1:D:203:ASP:O	1:D:204:TYR:C	2.56	0.44
1:E:167:PHE:HA	1:E:168:PRO:HD3	1.88	0.44
1:F:135:LEU:HD23	1:F:136:GLY:N	2.33	0.44
1:F:203:ASP:O	1:F:204:TYR:C	2.55	0.44
1:L:142:ILE:HG12	1:L:142:ILE:O	2.18	0.44
1:C:1:MET:SD	1:C:2:GLN:HG2	2.58	0.44
1:H:122:GLY:O	1:H:123:SER:HB2	2.18	0.44
1:M:118:ARG:HB3	1:M:125:ASP:HB2	1.99	0.44
1:G:265:ILE:HD13	1:G:277:VAL:HG21	1.99	0.44
1:H:192:ALA:O	6:H:323:PEG:H21	2.18	0.44
1:N:291:LYS:HE3	1:N:307:GLU:OE1	2.17	0.44
1:E:174:ARG:HD2	1:E:316:LEU:O	2.18	0.44
1:E:273:PRO:HA	1:E:274:PRO:HD3	1.94	0.44
1:F:254:ALA:HB1	1:F:284:LEU:HD23	2.00	0.44
1:G:258:LYS:HA	1:G:258:LYS:HD3	1.82	0.44
1:A:281:TYR:CE1	1:A:288:LYS:HD2	2.53	0.44
1:N:60:THR:HG22	1:N:70:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:167:PHE:HA	1:N:168:PRO:HD3	1.85	0.44
1:L:205:PRO:HD2	1:L:277:VAL:HG13	2.00	0.44
1:F:313:GLN:HA	1:F:317:LEU:HB2	2.00	0.43
1:I:2:GLN:HB2	1:I:3:LEU:H	1.61	0.43
1:B:139:THR:HG21	1:B:228:TYR:HB2	2.00	0.43
1:L:203:ASP:O	1:L:204:TYR:C	2.56	0.43
1:B:198:LYS:O	1:B:260:PRO:HD2	2.18	0.43
1:C:118:ARG:HB3	1:C:125:ASP:HB2	2.01	0.43
1:C:265:ILE:HD13	1:C:277:VAL:HG21	2.00	0.43
1:E:98:GLY:O	1:E:102:ILE:HG12	2.18	0.43
1:F:87:ARG:HD2	7:F:908:HOH:O	2.18	0.43
1:M:128:VAL:CG1	1:M:129:THR:N	2.80	0.43
1:B:165:GLN:NE2	7:B:384:HOH:O	2.48	0.43
1:M:7:SER:OG	1:M:10:GLU:HG3	2.18	0.43
1:M:225:ILE:HG22	1:M:229:PHE:CE2	2.53	0.43
1:N:231:ARG:HG3	1:N:231:ARG:HH11	1.83	0.43
1:A:135:LEU:HD21	1:F:136:GLY:HA2	1.99	0.43
1:A:167:PHE:HB3	1:A:169:GLU:OE1	2.19	0.43
1:E:165:GLN:HG3	1:E:172:GLU:CB	2.49	0.43
1:F:172:GLU:HG2	7:F:753:HOH:O	2.18	0.43
1:G:143:LEU:HD21	1:G:237:VAL:HG13	2.00	0.43
1:H:197:PRO:HG2	1:H:259:GLN:NE2	2.33	0.43
1:N:203:ASP:O	1:N:204:TYR:C	2.57	0.43
1:A:1:MET:N	1:A:270:LYS:HZ2	2.14	0.43
1:A:15:LYS:HD3	7:A:731:HOH:O	2.17	0.43
1:H:136:GLY:HA2	1:L:135:LEU:CD2	2.48	0.43
1:D:122:GLY:O	1:D:123:SER:HB2	2.19	0.43
1:H:139:THR:HG21	1:H:228:TYR:HB2	2.01	0.43
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.83	0.43
1:G:98:GLY:O	1:G:102:ILE:HG12	2.19	0.43
1:A:173:HIS:HB2	7:A:1424:HOH:O	2.18	0.43
1:C:102:ILE:HD11	1:C:114:GLY:HA3	2.00	0.43
1:C:177:VAL:CG2	1:C:200:VAL:HG22	2.49	0.43
1:H:196:ILE:N	1:H:197:PRO:HD2	2.34	0.43
1:D:55:LYS:HE3	1:D:55:LYS:HB2	1.92	0.42
1:N:198:LYS:O	1:N:259:GLN:HB3	2.19	0.42
1:B:26:ASP:OD2	1:B:30:LYS:HE3	2.18	0.42
1:G:63:SER:OG	1:G:64:PHE:N	2.51	0.42
1:L:59:LEU:HD23	1:L:113:PHE:CD1	2.54	0.42
1:M:198:LYS:O	1:M:259:GLN:HB3	2.19	0.42
1:M:212:ARG:HE	1:M:275:SER:CB	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PRO:O	1:B:259:GLN:HG2	2.18	0.42
1:I:44:LEU:HD12	1:I:44:LEU:HA	1.90	0.42
1:I:63:SER:OG	1:I:64:PHE:N	2.51	0.42
1:M:264:ALA:HB2	1:M:304:PHE:CZ	2.54	0.42
1:B:1:MET:O	1:B:2:GLN:O	2.38	0.42
1:F:161:LEU:HD13	1:F:197:PRO:HD3	2.02	0.42
1:I:21:ARG:CZ	1:I:243:GLU:HG2	2.48	0.42
1:I:136:GLY:HA2	1:N:135:LEU:HD11	2.00	0.42
1:M:88:PHE:HB3	1:M:186:LEU:HD12	2.02	0.42
1:N:98:GLY:O	1:N:102:ILE:HG12	2.19	0.42
1:A:273:PRO:HA	1:A:274:PRO:HD3	1.90	0.42
1:D:128:VAL:CG1	1:D:129:THR:N	2.82	0.42
1:A:126:THR:HA	1:F:128:VAL:HG13	2.00	0.42
1:C:234:ASP:HB3	1:C:237:VAL:CG2	2.49	0.42
1:F:201:VAL:HG11	1:F:308:LYS:HG3	2.02	0.42
1:I:136:GLY:HA2	1:N:135:LEU:CD1	2.49	0.42
1:I:78:GLN:HE21	1:I:78:GLN:HB3	1.62	0.42
1:B:118:ARG:HB3	1:B:125:ASP:HB2	2.01	0.42
1:G:220:GLN:HB3	1:G:221:PRO:HA	2.02	0.42
1:H:84:ALA:HB3	1:H:175:ILE:HG12	2.02	0.42
1:H:229:PHE:CE1	1:H:238:GLU:HA	2.55	0.42
1:I:59:LEU:HD12	1:I:60:THR:H	1.84	0.42
1:I:118:ARG:HB3	1:I:125:ASP:HB2	2.02	0.42
1:D:264:ALA:HB2	1:D:304:PHE:CZ	2.55	0.42
1:F:198:LYS:O	1:F:259:GLN:HB3	2.20	0.42
1:H:21:ARG:NH1	1:H:21:ARG:CG	2.83	0.42
1:M:117:VAL:HA	7:M:327:HOH:O	2.20	0.42
1:M:212:ARG:HG3	1:M:212:ARG:HH11	1.85	0.42
1:A:2:GLN:HG3	1:A:3:LEU:N	2.35	0.42
1:E:229:PHE:CE1	1:E:238:GLU:HA	2.55	0.42
1:L:16:PRO:HA	7:L:678:HOH:O	2.20	0.42
1:N:198:LYS:O	1:N:260:PRO:HD2	2.20	0.42
1:I:161:LEU:CD1	1:I:197:PRO:HG3	2.50	0.41
1:L:258:LYS:HA	1:L:258:LYS:HD3	1.83	0.41
1:L:273:PRO:HA	1:L:274:PRO:HD3	1.94	0.41
1:A:139:THR:HG21	1:A:228:TYR:HB2	2.02	0.41
1:B:236:LYS:HB2	1:B:236:LYS:HE2	1.87	0.41
1:L:265:ILE:HD13	1:L:277:VAL:HG21	2.01	0.41
1:M:1:MET:N	1:M:270:LYS:CE	2.83	0.41
1:A:4:PHE:CD1	1:A:270:LYS:HE3	2.55	0.41
1:F:164:ILE:HD13	1:F:167:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:VAL:CG1	1:H:129:THR:N	2.83	0.41
1:I:128:VAL:HG12	1:I:129:THR:N	2.35	0.41
1:L:201:VAL:HG11	1:L:308:LYS:HG3	2.02	0.41
1:B:135:LEU:CD2	1:D:135:LEU:HD22	2.50	0.41
1:D:69:ILE:N	1:D:69:ILE:CD1	2.83	0.41
1:G:128:VAL:CG1	1:G:129:THR:N	2.83	0.41
1:H:21:ARG:HG3	1:H:21:ARG:HH11	1.85	0.41
1:B:61:TYR:CD2	1:B:159:ARG:HG3	2.55	0.41
1:B:165:GLN:HB3	7:B:1406:HOH:O	2.20	0.41
1:F:196:ILE:N	1:F:197:PRO:HD2	2.35	0.41
1:N:92:ASN:ND2	7:N:345:HOH:O	2.50	0.41
1:N:128:VAL:O	1:N:130:PRO:HD3	2.21	0.41
1:M:21:ARG:HD3	1:M:247:TYR:OH	2.20	0.41
1:A:249:ASP:OD1	1:A:251:ILE:HG12	2.21	0.41
1:C:87:ARG:CG	4:C:323:PGE:H3	2.47	0.41
1:N:33:GLU:OE2	1:N:36:ARG:NH2	2.52	0.41
1:A:135:LEU:HD22	1:F:135:LEU:HD23	2.02	0.41
1:D:13:LYS:HG3	7:D:1465:HOH:O	2.20	0.41
1:E:139:THR:HG21	1:E:228:TYR:HB2	2.01	0.41
1:F:198:LYS:O	1:F:260:PRO:HD2	2.21	0.41
1:H:55:LYS:HE2	1:H:57:TYR:OH	2.20	0.41
1:N:220:GLN:HB3	1:N:221:PRO:HA	2.03	0.41
1:A:128:VAL:HG12	1:A:129:THR:N	2.35	0.41
1:E:317:LEU:HD12	1:E:317:LEU:HA	1.92	0.41
1:G:18:LYS:HE3	1:G:252:ASN:HA	2.01	0.41
1:N:178:ILE:HG22	1:N:201:VAL:HB	2.03	0.41
1:B:196:ILE:HB	1:B:197:PRO:HD3	2.02	0.41
1:D:141:GLY:HA2	2:D:322:CL:CL	2.58	0.41
1:E:220:GLN:O	1:E:271:ILE:HG23	2.21	0.41
1:H:267:LEU:HD23	1:H:267:LEU:HA	1.82	0.41
1:M:268:ILE:HG12	1:M:296:PHE:O	2.21	0.41
1:A:1:MET:N	1:A:270:LYS:HZ1	2.16	0.40
1:B:128:VAL:CG1	1:B:129:THR:N	2.84	0.40
1:B:128:VAL:O	1:B:130:PRO:HD3	2.21	0.40
1:B:145:LYS:HD3	1:B:247:TYR:CZ	2.55	0.40
1:C:139:THR:HG21	1:C:228:TYR:HB2	2.03	0.40
1:E:165:GLN:HG3	1:E:172:GLU:HB2	2.03	0.40
1:H:126:THR:HA	1:L:128:VAL:HG13	2.02	0.40
1:L:160:ALA:O	1:L:164:ILE:HG12	2.22	0.40
1:N:128:VAL:CG1	1:N:129:THR:N	2.84	0.40
1:E:229:PHE:CZ	1:E:238:GLU:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:LEU:HA	1:F:11:LEU:HD12	2.03	0.40
1:N:52:LYS:HA	7:N:1073:HOH:O	2.20	0.40
1:N:219:GLU:OE2	1:N:270:LYS:NZ	2.54	0.40
1:D:98:GLY:O	1:D:102:ILE:HG12	2.21	0.40
1:F:289:ASP:OD2	1:F:291:LYS:HE2	2.22	0.40
1:I:167:PHE:HB3	1:I:169:GLU:OE1	2.21	0.40
1:N:141:GLY:HA2	2:N:321:CL:CL	2.58	0.40
1:B:212:ARG:HH11	1:B:212:ARG:HG3	1.85	0.40
1:E:271:ILE:HD12	1:E:298:HIS:CD2	2.56	0.40
1:H:273:PRO:HA	1:H:274:PRO:HD3	1.94	0.40
1:L:33:GLU:OE2	1:L:36:ARG:NH2	2.54	0.40
1:N:143:LEU:HD23	1:N:143:LEU:HA	1.84	0.40
1:C:174:ARG:HD2	1:C:316:LEU:O	2.20	0.40
1:I:220:GLN:HB3	1:I:221:PRO:HA	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	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
1	B	316/320 (99%)	299 (95%)	16 (5%)	1 (0%)	41	61
1	C	318/320 (99%)	301 (95%)	16 (5%)	1 (0%)	41	61
1	D	316/320 (99%)	300 (95%)	15 (5%)	1 (0%)	41	61
1	E	316/320 (99%)	302 (96%)	13 (4%)	1 (0%)	41	61
1	F	315/320 (98%)	300 (95%)	15 (5%)	0	100	100
1	G	315/320 (98%)	299 (95%)	16 (5%)	0	100	100
1	H	315/320 (98%)	297 (94%)	18 (6%)	0	100	100
1	I	317/320 (99%)	300 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	315/320 (98%)	300 (95%)	15 (5%)	0	100 100
1	M	316/320 (99%)	299 (95%)	16 (5%)	1 (0%)	41 61
1	N	315/320 (98%)	301 (96%)	14 (4%)	0	100 100
All	All	3792/3840 (99%)	3601 (95%)	186 (5%)	5 (0%)	51 73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	GLN
1	D	2	GLN
1	E	2	GLN
1	M	2	GLN
1	C	2	GLN

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	270/270 (100%)	266 (98%)	4 (2%)	65 85
1	B	268/270 (99%)	265 (99%)	3 (1%)	73 89
1	C	270/270 (100%)	265 (98%)	5 (2%)	57 80
1	D	268/270 (99%)	267 (100%)	1 (0%)	91 97
1	E	268/270 (99%)	263 (98%)	5 (2%)	57 80
1	F	267/270 (99%)	264 (99%)	3 (1%)	73 89
1	G	267/270 (99%)	264 (99%)	3 (1%)	73 89
1	H	267/270 (99%)	263 (98%)	4 (2%)	65 85
1	I	269/270 (100%)	264 (98%)	5 (2%)	57 80
1	L	267/270 (99%)	263 (98%)	4 (2%)	65 85
1	M	268/270 (99%)	265 (99%)	3 (1%)	73 89
1	N	267/270 (99%)	263 (98%)	4 (2%)	65 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3216/3240 (99%)	3172 (99%)	44 (1%)	67 86

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	13	LYS
1	A	135	LEU
1	A	212	ARG
1	B	79	THR
1	B	135	LEU
1	B	236	LYS
1	C	1	MET
1	C	26	ASP
1	C	37	GLN
1	C	164	ILE
1	C	287	ASP
1	D	135	LEU
1	E	1	MET
1	E	3	LEU
1	E	35	LEU
1	E	78	GLN
1	E	287	ASP
1	F	37	GLN
1	F	165	GLN
1	F	203	ASP
1	G	3	LEU
1	G	203	ASP
1	G	219	GLU
1	H	3	LEU
1	H	21	ARG
1	H	44	LEU
1	H	310	SER
1	I	21	ARG
1	I	44	LEU
1	I	78	GLN
1	I	203	ASP
1	I	219	GLU
1	L	3	LEU
1	L	37	GLN
1	L	44	LEU
1	L	203	ASP

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Mol	Chain	Res	Type
1	M	26	ASP
1	M	48	ASP
1	M	79	THR
1	N	3	LEU
1	N	48	ASP
1	N	172	GLU
1	N	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	313	GLN
1	B	78	GLN
1	C	232	ASN
1	D	78	GLN
1	D	82	HIS
1	E	37	GLN
1	E	78	GLN
1	E	165	GLN
1	E	232	ASN
1	F	78	GLN
1	F	165	GLN
1	G	78	GLN
1	G	82	HIS
1	G	220	GLN
1	G	232	ASN
1	H	78	GLN
1	H	165	GLN
1	H	220	GLN
1	H	232	ASN
1	I	78	GLN
1	I	232	ASN
1	L	78	GLN
1	M	78	GLN
1	M	220	GLN
1	M	313	GLN
1	N	78	GLN
1	N	92	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 37 ligands modelled in this entry, 24 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	PG4	G	321	-	12,12,12	0.53	0	11,11,11	0.50	0
4	PGE	C	323	-	9,9,9	0.54	0	8,8,8	0.39	0
5	PG4	D	321	-	12,12,12	0.53	0	11,11,11	0.40	0
6	PEG	H	323	-	6,6,6	0.53	0	5,5,5	0.46	0
3	GOL	L	321	-	5,5,5	0.30	0	5,5,5	0.26	0
3	GOL	C	321	-	5,5,5	0.33	0	5,5,5	0.23	0
3	GOL	I	321	-	5,5,5	0.33	0	5,5,5	0.32	0
5	PG4	H	322	-	12,12,12	0.54	0	11,11,11	0.44	0
6	PEG	M	321	-	6,6,6	0.53	0	5,5,5	0.35	0
3	GOL	C	322	-	5,5,5	0.32	0	5,5,5	0.23	0
6	PEG	H	321	-	6,6,6	0.53	0	5,5,5	0.41	0
3	GOL	F	321	-	5,5,5	0.32	0	5,5,5	0.23	0
4	PGE	F	322	-	9,9,9	0.53	0	8,8,8	0.40	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
5	PG4	G	321	-	-	0/10/10/10	-
4	PGE	C	323	-	-	0/7/7/7	-
5	PG4	D	321	-	-	4/10/10/10	-
6	PEG	H	323	-	-	0/4/4/4	-
3	GOL	L	321	-	-	0/4/4/4	-
3	GOL	C	321	-	-	0/4/4/4	-
3	GOL	I	321	-	-	0/4/4/4	-
5	PG4	H	322	-	-	1/10/10/10	-
6	PEG	M	321	-	-	1/4/4/4	-
3	GOL	C	322	-	-	0/4/4/4	-
6	PEG	H	321	-	-	0/4/4/4	-
3	GOL	F	321	-	-	0/4/4/4	-
4	PGE	F	322	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	322	PGE	C3-C4-O3-C5
6	M	321	PEG	C4-C3-O2-C2
5	D	321	PG4	C4-C3-O2-C2
5	D	321	PG4	C1-C2-O2-C3
5	D	321	PG4	C3-C4-O3-C5
5	D	321	PG4	O2-C3-C4-O3
5	H	322	PG4	O3-C5-C6-O4
4	F	322	PGE	O2-C3-C4-O3

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	321	PG4	1	0
4	C	323	PGE	9	0
6	H	323	PEG	1	0
5	H	322	PG4	8	0
6	M	321	PEG	6	0
3	C	322	GOL	1	0
6	H	321	PEG	1	0
4	F	322	PGE	2	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

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	320/320 (100%)	-0.37	3 (0%)	84	86	5, 14, 27, 49	0
1	B	318/320 (99%)	-0.30	1 (0%)	94	94	7, 17, 29, 46	0
1	C	320/320 (100%)	-0.24	2 (0%)	89	90	9, 18, 31, 43	0
1	D	318/320 (99%)	-0.23	5 (1%)	72	74	10, 18, 32, 44	0
1	E	318/320 (99%)	-0.25	4 (1%)	77	79	8, 17, 29, 53	0
1	F	317/320 (99%)	-0.25	2 (0%)	89	90	7, 16, 29, 44	0
1	G	317/320 (99%)	-0.21	4 (1%)	77	79	8, 17, 30, 46	0
1	H	317/320 (99%)	-0.24	1 (0%)	94	94	8, 16, 29, 40	0
1	I	319/320 (99%)	-0.20	5 (1%)	72	74	8, 17, 32, 54	0
1	L	317/320 (99%)	-0.24	2 (0%)	89	90	9, 18, 31, 43	0
1	M	318/320 (99%)	-0.17	4 (1%)	77	79	8, 18, 31, 46	0
1	N	317/320 (99%)	-0.26	2 (0%)	89	90	9, 16, 28, 44	0
All	All	3816/3840 (99%)	-0.25	35 (0%)	84	86	5, 17, 30, 54	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	318	LEU	5.7
1	E	1	MET	4.7
1	I	1	MET	4.6
1	C	320	THR	3.6
1	A	1	MET	3.4
1	F	318	LEU	3.2
1	B	318	LEU	3.0
1	L	79	THR	3.0
1	G	318	LEU	3.0
1	L	318	LEU	2.8
1	E	318	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	79	THR	2.7
1	A	320	THR	2.5
1	G	317	LEU	2.5
1	C	79	THR	2.5
1	I	2	GLN	2.4
1	H	186	LEU	2.4
1	M	10	GLU	2.4
1	M	185	ALA	2.4
1	G	36	ARG	2.3
1	F	79	THR	2.2
1	D	1	MET	2.2
1	D	287	ASP	2.2
1	E	36	ARG	2.2
1	D	79	THR	2.2
1	E	79	THR	2.2
1	N	287	ASP	2.1
1	D	86	VAL	2.1
1	I	79	THR	2.1
1	I	78	GLN	2.1
1	I	77	ASP	2.1
1	N	80	GLY	2.1
1	D	45	GLU	2.1
1	G	78	GLN	2.0
1	M	81	PRO	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, 95^{th} 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
3	GOL	I	321	6/6	0.64	0.27	35,37,38,39	0
3	GOL	L	321	6/6	0.69	0.27	36,38,39,40	0
3	GOL	C	321	6/6	0.74	0.32	32,35,35,35	0
5	PG4	D	321	13/13	0.77	0.29	49,51,55,57	0
5	PG4	G	321	13/13	0.77	0.33	42,44,49,50	0
4	PGE	F	322	10/10	0.80	0.32	49,51,53,53	0
6	PEG	H	323	7/7	0.81	0.20	58,59,62,62	0
4	PGE	C	323	10/10	0.83	0.28	42,47,51,51	0
3	GOL	F	321	6/6	0.84	0.26	27,31,32,33	0
3	GOL	C	322	6/6	0.85	0.25	30,32,33,33	0
5	PG4	H	322	13/13	0.87	0.26	47,54,56,56	0
6	PEG	M	321	7/7	0.90	0.21	32,36,39,42	0
6	PEG	H	321	7/7	0.92	0.25	30,30,32,34	0
2	CL	C	325	1/1	0.96	0.08	32,32,32,32	0
2	CL	I	323	1/1	0.96	0.09	28,28,28,28	0
2	CL	B	322	1/1	0.96	0.05	26,26,26,26	0
2	CL	E	321	1/1	0.97	0.11	23,23,23,23	0
2	CL	H	325	1/1	0.97	0.07	35,35,35,35	0
2	CL	D	322	1/1	0.97	0.08	25,25,25,25	0
2	CL	L	323	1/1	0.97	0.05	36,36,36,36	0
2	CL	M	323	1/1	0.97	0.07	41,41,41,41	0
2	CL	D	323	1/1	0.97	0.08	34,34,34,34	0
2	CL	N	322	1/1	0.98	0.06	33,33,33,33	0
2	CL	B	321	1/1	0.98	0.10	27,27,27,27	0
2	CL	I	322	1/1	0.98	0.06	25,25,25,25	0
2	CL	A	321	1/1	0.98	0.07	16,16,16,16	0
2	CL	L	322	1/1	0.98	0.07	24,24,24,24	0
2	CL	F	324	1/1	0.98	0.06	32,32,32,32	0
2	CL	G	323	1/1	0.98	0.10	31,31,31,31	0
2	CL	A	322	1/1	0.99	0.04	29,29,29,29	0
2	CL	G	322	1/1	0.99	0.10	24,24,24,24	0
2	CL	E	322	1/1	0.99	0.05	30,30,30,30	0
2	CL	H	324	1/1	0.99	0.07	22,22,22,22	0
2	CL	M	322	1/1	0.99	0.06	21,21,21,21	0
2	CL	F	323	1/1	0.99	0.07	20,20,20,20	0
2	CL	N	321	1/1	0.99	0.06	23,23,23,23	0
2	CL	C	324	1/1	1.00	0.06	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.