



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2016 – 12:29 PM EDT

PDB ID : 5AYE
Title : Crystal structure of Ruminococcus albus beta-(1,4)-mannooligosaccharide phosphorylase (RaMP2) in complexes with phosphate and beta-(1,4)-mannobiose
Authors : Ye, Y.; Saburi, W.; Kato, K.; Yao, M.
Deposited on : 2015-08-13
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

i

X-RAY DIFFRACTION

A.



R_{free}
Clashscore
Ramachandran outliers
Sidechain outliers
RSRZ outliers

electron density. The numeric value is given above the bar.

1	A	335
1	B	335
1	C	335
1	D	335
1	E	335
1	F	335

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	PO4	C	401	-	X	-	-
3	BMA	A	402	-	-	-	X
3	BMA	A	403	-	-	-	X
3	BMA	B	402	-	-	-	X
3	BMA	B	403	-	-	-	X
3	BMA	C	402	-	-	-	X
3	BMA	C	403	-	-	-	X
3	BMA	D	402	-	-	-	X
3	BMA	D	403	-	-	-	X
3	BMA	E	402	-	-	-	X
3	BMA	E	403	-	-	-	X
3	BMA	F	402	-	-	-	X
3	BMA	F	403	-	-	-	X

2 Entry composition [i](#)

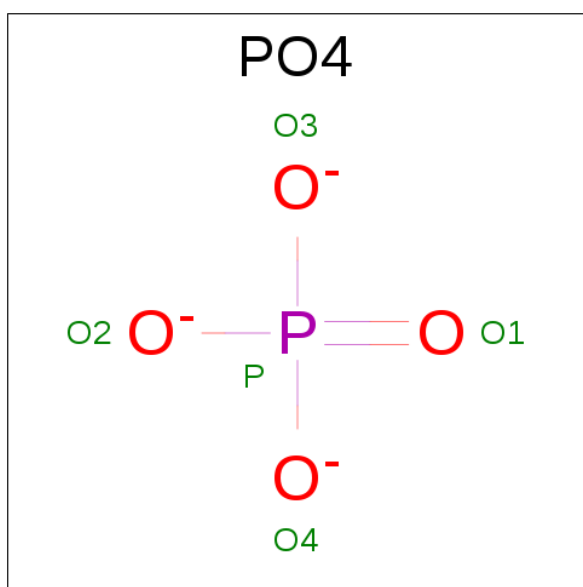
There are 4 unique types of molecules in this entry. The entry contains 17797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-1,4-mannooligosaccharide phosphorylase.

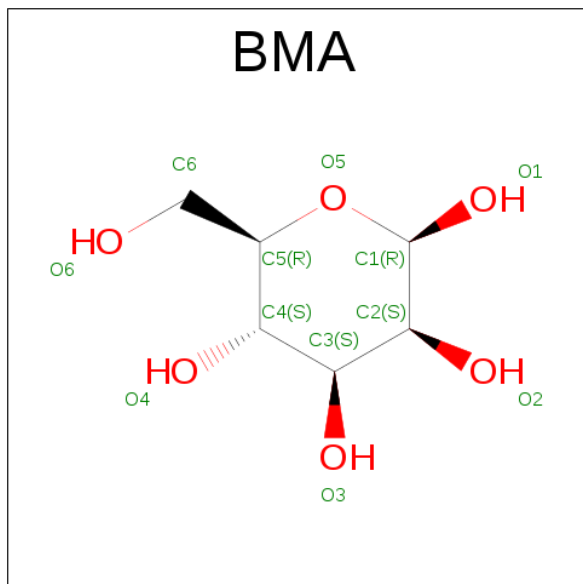
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2700	1737	446	497	20			
1	B	335	Total	C	N	O	S	0	0	0
			2700	1737	446	497	20			
1	C	335	Total	C	N	O	S	0	0	0
			2700	1737	446	497	20			
1	D	335	Total	C	N	O	S	0	0	0
			2700	1737	446	497	20			
1	E	335	Total	C	N	O	S	0	0	0
			2700	1737	446	497	20			
1	F	335	Total	C	N	O	S	0	0	0
			2700	1737	446	497	20			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 12 6 6	0	0
3	B	1	Total C O 11 6 5	0	0
3	C	1	Total C O 12 6 6	0	0
3	C	1	Total C O 11 6 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			11	6	5		
3	E	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			11	6	5		
3	F	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			11	6	5		

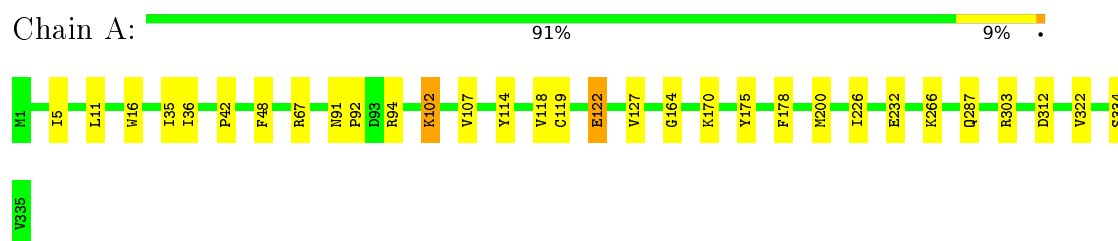
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		
4	B	224	Total	O	0	0
			224	224		
4	C	251	Total	O	0	0
			251	251		
4	D	226	Total	O	0	0
			226	226		
4	E	222	Total	O	0	0
			222	222		
4	F	286	Total	O	0	0
			286	286		

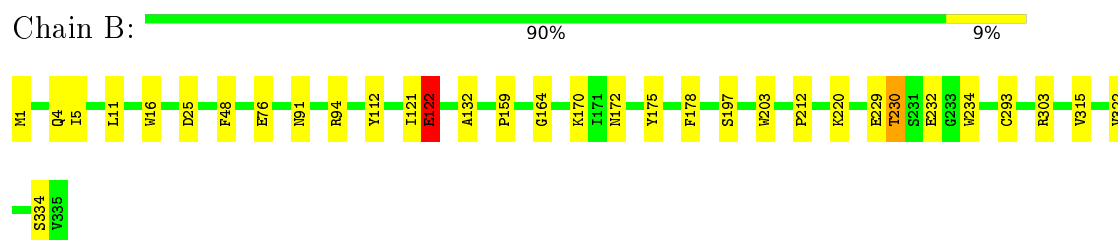
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

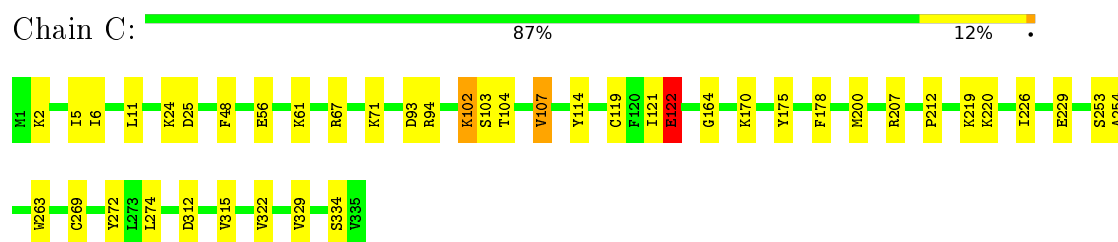
- Molecule 1: Beta-1,4-mannooligosaccharide phosphorylase



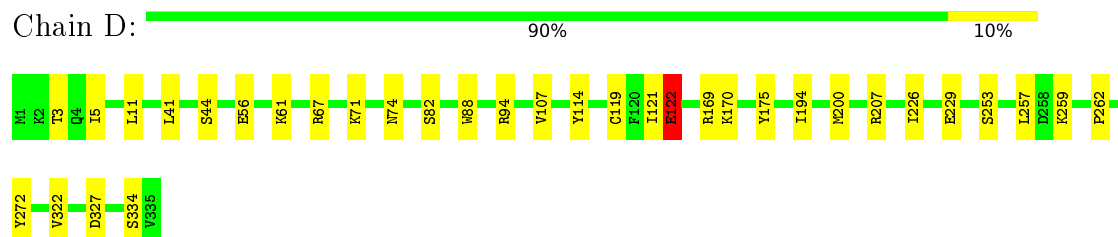
- Molecule 1: Beta-1,4-mannooligosaccharide phosphorylase



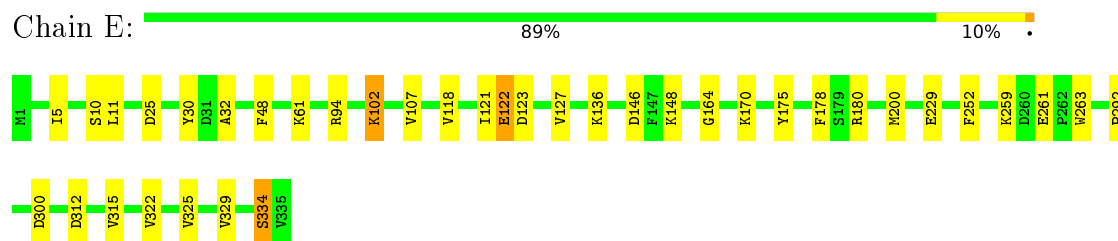
- Molecule 1: Beta-1,4-mannooligosaccharide phosphorylase



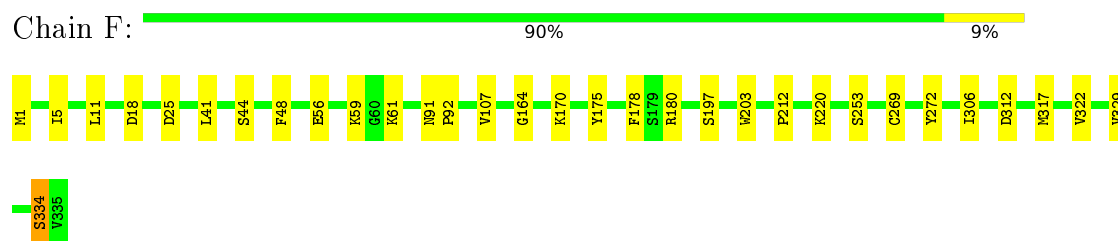
- Molecule 1: Beta-1,4-mannooligosaccharide phosphorylase



- Molecule 1: Beta-1,4-mannooligosaccharide phosphorylase



- Molecule 1: Beta-1,4-mannooligosaccharide phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.47Å 166.15Å 92.72Å 90.00° 118.87° 90.00°	Depositor
Resolution (Å)	47.09 – 2.20 47.09 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.09-2.20) 99.1 (47.09-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.166 , 0.213 0.166 , 0.213	Depositor DCC
R_{free} test set	6187 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.6	EDS
Estimated twinning fraction	0.034 for -h-l,k,h 0.034 for l,k,-h-l 0.044 for h,-k,-h-l 0.039 for -h-l,-k,l 0.196 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 123748 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17797	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, BMA

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	0.41	0/2787	0.54	0/3791
1	B	0.42	0/2787	0.54	0/3791
1	C	0.44	0/2787	0.54	0/3791
1	D	0.41	0/2787	0.52	0/3791
1	E	0.42	0/2787	0.53	0/3791
1	F	0.42	0/2787	0.54	0/3791
All	All	0.42	0/16722	0.53	0/22746

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 [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	2700	0	2564	18	0
1	B	2700	0	2564	24	0
1	C	2700	0	2564	29	0
1	D	2700	0	2564	20	0
1	E	2700	0	2564	24	0
1	F	2700	0	2564	18	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	23	0	21	0	0
3	B	23	0	21	0	0
3	C	23	0	21	0	0
3	D	23	0	21	0	0
3	E	23	0	21	0	0
3	F	23	0	21	0	0
4	A	220	0	0	1	0
4	B	224	0	0	8	0
4	C	251	0	0	6	0
4	D	226	0	0	5	0
4	E	222	0	0	5	0
4	F	286	0	0	5	0
All	All	17797	0	15510	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (128) 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:E:146:ASP:OD2	4:E:501:HOH:O	1.88	0.92
1:C:263:TRP:O	4:C:501:HOH:O	1.89	0.89
1:D:5:ILE:HD11	1:D:322:VAL:HG21	1.56	0.88
1:E:122:GLU:OE2	4:E:502:HOH:O	2.00	0.80
1:C:5:ILE:HD11	1:C:322:VAL:HG21	1.69	0.74
1:F:5:ILE:HD11	1:F:322:VAL:HG21	1.68	0.74
1:C:207:ARG:CZ	1:F:107:VAL:HG21	2.21	0.71
1:B:5:ILE:HD11	1:B:322:VAL:HG21	1.73	0.70
1:D:327:ASP:OD1	4:D:502:HOH:O	2.09	0.69
1:A:5:ILE:HD11	1:A:322:VAL:HG21	1.74	0.69
1:C:93:ASP:OD1	4:C:502:HOH:O	2.13	0.66
1:B:76:GLU:OE2	4:B:501:HOH:O	2.14	0.66
1:E:5:ILE:HD11	1:E:322:VAL:HG21	1.77	0.66
1:A:35:ILE:HG13	1:A:36:ILE:HG13	1.78	0.65
1:D:67:ARG:HD2	1:D:114:TYR:HB2	1.80	0.64
1:F:18:ASP:OD1	4:F:501:HOH:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ARG:NH1	4:D:501:HOH:O	1.92	0.61
1:A:102:LYS:NZ	1:A:102:LYS:H	2.03	0.57
1:F:56:GLU:OE2	1:F:61:LYS:NZ	2.25	0.57
1:E:102:LYS:NZ	1:E:102:LYS:H	2.03	0.56
1:B:4:GLN:OE1	4:B:502:HOH:O	2.18	0.56
1:C:25:ASP:HB3	4:C:583:HOH:O	2.05	0.56
1:C:253:SER:HB2	1:C:272:TYR:HA	1.88	0.56
1:E:94:ARG:NH2	4:E:506:HOH:O	2.35	0.56
1:D:170:LYS:HE2	1:D:175:TYR:CZ	2.40	0.56
1:C:103:SER:HB2	4:F:532:HOH:O	2.06	0.55
1:C:6:ILE:HB	1:C:229:GLU:HG2	1.89	0.55
1:C:56:GLU:OE2	1:C:61:LYS:NZ	2.26	0.55
1:F:59:LYS:NZ	4:F:510:HOH:O	2.40	0.55
1:C:119:CYS:HB3	1:C:226:ILE:HG13	1.88	0.54
1:F:107:VAL:HG23	4:F:504:HOH:O	2.06	0.54
1:C:170:LYS:HE2	1:C:175:TYR:CZ	2.43	0.54
1:E:170:LYS:HE2	1:E:175:TYR:CZ	2.43	0.53
1:D:121:ILE:O	1:D:122:GLU:HG2	2.08	0.53
1:C:102:LYS:CD	1:C:102:LYS:H	2.22	0.53
1:E:118:VAL:HG22	1:E:127:VAL:HG22	1.90	0.53
1:E:48:PHE:HA	1:E:315:VAL:HG22	1.91	0.52
1:A:175:TYR:CD2	1:A:200:MET:HG2	2.45	0.52
1:A:102:LYS:HZ3	1:A:102:LYS:H	1.57	0.52
1:A:94:ARG:NH2	4:A:517:HOH:O	2.42	0.52
1:B:25:ASP:HB3	4:B:566:HOH:O	2.10	0.52
1:B:94:ARG:NH2	4:B:508:HOH:O	2.42	0.52
1:D:94:ARG:HD3	4:D:681:HOH:O	2.09	0.51
1:A:42:PRO:HA	1:C:24:LYS:HD2	1.93	0.51
1:B:170:LYS:HE2	1:B:175:TYR:CZ	2.45	0.51
1:B:121:ILE:O	1:B:122:GLU:HG2	2.11	0.50
1:D:119:CYS:HB3	1:D:226:ILE:HG13	1.92	0.50
1:F:170:LYS:HE2	1:F:175:TYR:CZ	2.46	0.50
1:D:56:GLU:OE2	1:D:61:LYS:NZ	2.26	0.49
1:B:230:THR:HG22	1:B:232:GLU:H	1.76	0.49
1:C:269:CYS:HB2	1:C:329:VAL:HG22	1.94	0.49
1:D:194:ILE:HG13	1:D:207:ARG:HB2	1.94	0.49
1:F:41:LEU:HB2	1:F:44:SER:HB3	1.95	0.48
1:E:175:TYR:CD2	1:E:200:MET:HG2	2.47	0.48
1:D:229:GLU:OE2	1:D:259:LYS:NZ	2.41	0.48
1:D:74:ASN:HB3	4:D:644:HOH:O	2.13	0.48
1:C:175:TYR:CD2	1:C:200:MET:HG2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:THR:CG2	1:B:232:GLU:H	2.26	0.47
1:C:48:PHE:HA	1:C:315:VAL:HG22	1.95	0.47
1:E:121:ILE:O	1:E:123:ASP:N	2.42	0.47
1:A:170:LYS:HE2	1:A:175:TYR:CZ	2.50	0.47
1:C:2:LYS:NZ	4:C:515:HOH:O	2.47	0.47
1:E:102:LYS:H	1:E:102:LYS:HZ3	1.60	0.47
1:C:121:ILE:O	1:C:122:GLU:HG2	2.15	0.47
1:B:159:PRO:HD3	4:B:542:HOH:O	2.15	0.46
1:E:121:ILE:O	1:E:122:GLU:HG2	2.15	0.46
1:C:94:ARG:NH2	4:C:518:HOH:O	2.48	0.46
1:D:175:TYR:CD2	1:D:200:MET:HG2	2.51	0.46
1:D:3:THR:OG1	4:D:503:HOH:O	2.20	0.46
1:A:119:CYS:HB3	1:A:226:ILE:HG13	1.96	0.46
1:B:197:SER:HB2	1:B:203:TRP:CE3	2.51	0.45
1:B:212:PRO:HG3	1:B:220:LYS:HA	1.97	0.45
1:D:82:SER:HB2	1:D:88:TRP:CD2	2.51	0.45
1:B:25:ASP:OD1	1:C:71:LYS:NZ	2.49	0.45
1:F:253:SER:HB2	1:F:272:TYR:HA	1.98	0.45
1:E:10:SER:OG	1:E:300:ASP:OD2	2.17	0.45
1:E:252:PHE:CG	1:E:292:PRO:HG3	2.53	0.44
1:C:219:LYS:HA	1:C:219:LYS:HD3	1.88	0.44
1:F:25:ASP:HB3	4:F:528:HOH:O	2.17	0.44
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.87	0.44
1:C:212:PRO:HG3	1:C:220:LYS:HA	1.98	0.44
1:C:207:ARG:NE	1:F:107:VAL:HG21	2.32	0.44
1:E:229:GLU:OE2	1:E:259:LYS:NZ	2.37	0.43
1:E:325:VAL:O	1:E:329:VAL:HG23	2.18	0.43
1:B:164:GLY:HA2	1:B:178:PHE:O	2.18	0.43
1:C:67:ARG:HD2	1:C:114:TYR:HB2	2.01	0.43
1:D:257:LEU:HD13	1:D:262:PRO:O	2.19	0.43
1:D:121:ILE:C	1:D:122:GLU:HG2	2.38	0.43
1:D:41:LEU:HB2	1:D:44:SER:HB3	2.00	0.43
1:B:121:ILE:C	1:B:122:GLU:HG2	2.39	0.43
1:B:112:TYR:CZ	1:B:132:ALA:HB2	2.54	0.43
1:C:48:PHE:CD2	1:C:312:ASP:HA	2.52	0.43
1:E:61:LYS:NZ	4:E:521:HOH:O	2.52	0.43
1:E:136:LYS:NZ	4:E:509:HOH:O	2.39	0.43
1:B:91:ASN:HB3	4:B:642:HOH:O	2.17	0.43
1:E:164:GLY:HA2	1:E:178:PHE:O	2.18	0.43
1:A:164:GLY:HA2	1:A:178:PHE:O	2.18	0.42
1:D:253:SER:HB2	1:D:272:TYR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:LYS:NZ	1:E:25:ASP:OD1	2.51	0.42
1:E:48:PHE:CD2	1:E:312:ASP:HA	2.54	0.42
1:C:104:THR:HA	1:C:107:VAL:HG23	2.01	0.42
1:B:197:SER:HB2	1:B:203:TRP:CD2	2.55	0.42
1:E:30:TYR:CE2	1:E:32:ALA:HB3	2.53	0.42
1:F:91:ASN:HA	1:F:92:PRO:HD3	1.89	0.42
1:A:67:ARG:HD2	1:A:114:TYR:HB2	2.01	0.42
1:C:164:GLY:HA2	1:C:178:PHE:O	2.19	0.42
1:F:269:CYS:HB2	1:F:329:VAL:HG22	2.00	0.42
1:B:16:TRP:CH2	1:B:303:ARG:HG2	2.55	0.42
1:B:293:CYS:HB2	4:B:582:HOH:O	2.20	0.42
1:E:261:GLU:HB3	1:E:263:TRP:CZ2	2.55	0.42
1:A:232:GLU:O	1:A:266:LYS:NZ	2.38	0.42
1:F:212:PRO:HG3	1:F:220:LYS:HA	2.01	0.42
1:A:102:LYS:CE	1:A:102:LYS:H	2.33	0.41
1:C:102:LYS:NZ	4:C:523:HOH:O	2.53	0.41
1:A:16:TRP:CD2	1:A:303:ARG:HD2	2.55	0.41
1:F:197:SER:HB2	1:F:203:TRP:CD2	2.55	0.41
1:A:118:VAL:HG22	1:A:127:VAL:HG22	2.03	0.41
1:A:48:PHE:CD2	1:A:312:ASP:HA	2.55	0.41
1:B:112:TYR:CE1	1:B:132:ALA:HB2	2.55	0.41
1:F:164:GLY:HA2	1:F:178:PHE:O	2.20	0.41
1:B:229:GLU:HB2	1:B:234:TRP:CZ3	2.56	0.41
1:C:253:SER:OG	1:C:254:ALA:N	2.53	0.41
1:F:306:ILE:O	1:F:317:MET:HA	2.20	0.41
1:F:48:PHE:CD2	1:F:312:ASP:HA	2.56	0.40
1:B:76:GLU:HG3	4:B:563:HOH:O	2.21	0.40
1:E:148:LYS:HB2	1:E:148:LYS:HE3	1.76	0.40
1:A:5:ILE:CD1	1:A:322:VAL:HG21	2.47	0.40
1:B:48:PHE:HA	1:B:315:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	333/335 (99%)	314 (94%)	17 (5%)	2 (1%)	30	29
1	B	333/335 (99%)	316 (95%)	15 (4%)	2 (1%)	30	29
1	C	333/335 (99%)	319 (96%)	12 (4%)	2 (1%)	30	29
1	D	333/335 (99%)	313 (94%)	18 (5%)	2 (1%)	30	29
1	E	333/335 (99%)	314 (94%)	17 (5%)	2 (1%)	30	29
1	F	333/335 (99%)	309 (93%)	23 (7%)	1 (0%)	46	50
All	All	1998/2010 (99%)	1885 (94%)	102 (5%)	11 (1%)	30	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU
1	B	122	GLU
1	C	122	GLU
1	D	122	GLU
1	D	334	SER
1	E	122	GLU
1	B	334	SER
1	E	334	SER
1	F	334	SER
1	A	334	SER
1	C	334	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/294 (100%)	289 (98%)	5 (2%)	68	81
1	B	294/294 (100%)	289 (98%)	5 (2%)	68	81
1	C	294/294 (100%)	289 (98%)	5 (2%)	68	81
1	D	294/294 (100%)	291 (99%)	3 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	294/294 (100%)	289 (98%)	5 (2%)	68	81
1	F	294/294 (100%)	290 (99%)	4 (1%)	74	85
All	All	1764/1764 (100%)	1737 (98%)	27 (2%)	72	84

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	102	LYS
1	A	107	VAL
1	A	122	GLU
1	A	287	GLN
1	B	1	MET
1	B	11	LEU
1	B	122	GLU
1	B	172	ASN
1	B	230	THR
1	C	11	LEU
1	C	102	LYS
1	C	107	VAL
1	C	122	GLU
1	C	274	LEU
1	D	11	LEU
1	D	107	VAL
1	D	122	GLU
1	E	11	LEU
1	E	102	LYS
1	E	107	VAL
1	E	180	ARG
1	E	334	SER
1	F	1	MET
1	F	11	LEU
1	F	180	ARG
1	F	334	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	E	7	ASN

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Mol	Chain	Res	Type
1	F	332	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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$
2	PO4	A	401	-	4,4,4	0.60	0	6,6,6	0.23	0
3	BMA	A	402	3	12,12,12	0.93	1 (8%)	17,17,17	1.70	4 (23%)
3	BMA	A	403	3	11,11,12	1.03	0	15,15,17	3.74	7 (46%)
2	PO4	B	401	-	4,4,4	0.58	0	6,6,6	0.28	0
3	BMA	B	402	3	12,12,12	1.15	1 (8%)	17,17,17	1.00	1 (5%)
3	BMA	B	403	3	11,11,12	0.99	0	15,15,17	3.53	9 (60%)
2	PO4	C	401	-	4,4,4	3.51	4 (100%)	6,6,6	0.23	0
3	BMA	C	402	3	12,12,12	1.07	1 (8%)	17,17,17	2.28	6 (35%)
3	BMA	C	403	3	11,11,12	1.21	1 (9%)	15,15,17	3.34	8 (53%)
2	PO4	D	401	-	4,4,4	0.51	0	6,6,6	0.25	0
3	BMA	D	402	3	12,12,12	1.13	1 (8%)	17,17,17	1.70	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	D	403	3	11,11,12	0.78	0	15,15,17	3.67	10 (66%)
2	PO4	E	401	-	4,4,4	0.71	0	6,6,6	0.24	0
3	BMA	E	402	3	12,12,12	0.85	0	17,17,17	1.69	5 (29%)
3	BMA	E	403	3	11,11,12	1.15	1 (9%)	15,15,17	3.34	8 (53%)
2	PO4	F	401	-	4,4,4	0.71	0	6,6,6	0.24	0
3	BMA	F	402	3	12,12,12	1.19	1 (8%)	17,17,17	1.61	4 (23%)
3	BMA	F	403	3	11,11,12	0.75	0	15,15,17	3.40	7 (46%)

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
2	PO4	A	401	-	-	0/0/0/0	0/0/0/0
3	BMA	A	402	3	-	0/2/22/22	0/1/1/1
3	BMA	A	403	3	-	0/2/19/22	0/1/1/1
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
3	BMA	B	402	3	-	0/2/22/22	0/1/1/1
3	BMA	B	403	3	-	0/2/19/22	0/1/1/1
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0
3	BMA	C	402	3	-	0/2/22/22	0/1/1/1
3	BMA	C	403	3	-	0/2/19/22	0/1/1/1
2	PO4	D	401	-	-	0/0/0/0	0/0/0/0
3	BMA	D	402	3	-	0/2/22/22	0/1/1/1
3	BMA	D	403	3	-	0/2/19/22	0/1/1/1
2	PO4	E	401	-	-	0/0/0/0	0/0/0/0
3	BMA	E	402	3	-	0/2/22/22	0/1/1/1
3	BMA	E	403	3	-	0/2/19/22	1/1/1/1
2	PO4	F	401	-	-	0/0/0/0	0/0/0/0
3	BMA	F	402	3	-	0/2/22/22	0/1/1/1
3	BMA	F	403	3	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PO4	P-O3	-4.18	1.40	1.53
2	C	401	PO4	P-O4	-3.34	1.43	1.53
2	C	401	PO4	P-O1	-3.24	1.40	1.53
3	F	402	BMA	O5-C1	-3.21	1.36	1.43
2	C	401	PO4	P-O2	-3.16	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	BMA	O5-C1	-2.77	1.37	1.43
3	D	402	BMA	O5-C1	-2.75	1.37	1.43
3	A	402	BMA	O5-C1	-2.61	1.38	1.43
3	C	402	BMA	O5-C1	-2.47	1.38	1.43
3	E	403	BMA	C4-C3	2.22	1.58	1.52
3	C	403	BMA	C2-C3	3.27	1.56	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	403	BMA	C1-C2-C3	-6.67	101.47	109.55
3	B	403	BMA	C1-C2-C3	-6.47	101.71	109.55
3	D	403	BMA	C1-C2-C3	-6.40	101.80	109.55
3	A	403	BMA	C1-C2-C3	-5.82	102.50	109.55
3	E	403	BMA	C1-C2-C3	-5.71	102.63	109.55
3	C	402	BMA	O6-C6-C5	-5.11	94.24	111.30
3	C	403	BMA	C1-C2-C3	-5.10	103.38	109.55
3	D	403	BMA	O5-C1-C2	-4.90	103.05	110.89
3	A	403	BMA	O5-C1-C2	-4.86	103.13	110.89
3	B	403	BMA	O5-C1-C2	-4.69	103.40	110.89
3	C	402	BMA	C6-C5-C4	-4.00	102.97	112.99
3	F	403	BMA	O6-C6-C5	-3.77	98.72	111.30
3	D	402	BMA	O2-C2-C3	-3.74	101.93	110.36
3	D	403	BMA	O5-C5-C6	-3.54	99.76	107.34
3	E	402	BMA	O2-C2-C3	-3.50	102.47	110.36
3	C	403	BMA	O5-C1-C2	-3.43	105.42	110.89
3	C	403	BMA	C6-C5-C4	-3.35	104.60	112.99
3	D	403	BMA	O6-C6-C5	-3.20	100.63	111.30
3	F	402	BMA	C1-C2-C3	-3.16	105.50	110.68
3	E	403	BMA	O6-C6-C5	-3.04	101.16	111.30
3	A	402	BMA	O5-C5-C6	-3.03	98.54	106.38
3	E	402	BMA	C1-O5-C5	-2.97	107.86	113.54
3	B	403	BMA	O6-C6-C5	-2.77	102.06	111.30
3	F	403	BMA	O5-C1-C2	-2.73	106.53	110.89
3	D	402	BMA	O3-C3-C2	-2.48	104.77	110.36
3	D	402	BMA	O5-C5-C6	-2.31	100.39	106.38
3	A	402	BMA	O1-C1-O5	-2.25	104.06	110.33
3	E	403	BMA	O5-C5-C4	-2.08	106.70	110.13
3	C	402	BMA	O1-C1-O5	-2.07	104.56	110.33
3	E	403	BMA	O4-C4-C5	-2.05	103.82	109.23
3	C	402	BMA	O3-C3-C2	-2.05	105.74	110.36
3	A	403	BMA	O6-C6-C5	-2.05	104.47	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	BMA	O1-C1-C2	2.01	114.60	109.05
3	A	403	BMA	C3-C4-C5	2.05	113.88	110.23
3	E	402	BMA	C6-C5-C4	2.08	118.19	112.99
3	F	402	BMA	O1-C1-C2	2.08	114.80	109.05
3	E	402	BMA	O4-C4-C5	2.09	114.72	109.23
3	B	403	BMA	O5-C5-C4	2.11	113.62	110.13
3	D	403	BMA	O5-C5-C4	2.14	113.68	110.13
3	B	403	BMA	C3-C4-C5	2.18	114.12	110.23
3	D	403	BMA	C2-C3-C4	2.19	114.86	111.05
3	D	403	BMA	C3-C4-C5	2.22	114.19	110.23
3	F	402	BMA	O3-C3-C4	2.23	115.38	110.36
3	B	403	BMA	C2-C3-C4	2.36	115.17	111.05
3	B	402	BMA	O1-C1-C2	2.52	116.01	109.05
3	C	402	BMA	C1-O5-C5	2.52	118.37	113.54
3	E	403	BMA	C3-C4-C5	2.66	114.98	110.23
3	C	403	BMA	O5-C5-C4	2.70	114.61	110.13
3	D	403	BMA	O2-C2-C1	2.71	114.67	109.23
3	A	402	BMA	O1-C1-C2	2.79	116.75	109.05
3	F	403	BMA	C2-C3-C4	2.81	115.94	111.05
3	C	403	BMA	O2-C2-C1	2.84	114.93	109.23
3	C	403	BMA	C3-C4-C5	2.88	115.37	110.23
3	F	402	BMA	O4-C4-C3	2.92	116.95	110.36
3	E	402	BMA	O1-C1-C2	2.99	117.30	109.05
3	A	402	BMA	O4-C4-C5	3.10	117.41	109.23
3	F	403	BMA	O2-C2-C3	3.28	116.79	110.19
3	F	403	BMA	O2-C2-C1	3.59	116.41	109.23
3	A	403	BMA	O2-C2-C1	3.63	116.50	109.23
3	B	403	BMA	O2-C2-C1	3.67	116.58	109.23
3	E	403	BMA	O2-C2-C3	3.97	118.19	110.19
3	C	402	BMA	O5-C5-C4	4.14	117.56	109.67
3	D	403	BMA	O2-C2-C3	4.33	118.92	110.19
3	B	403	BMA	O2-C2-C3	4.59	119.44	110.19
3	E	403	BMA	O2-C2-C1	5.22	119.69	109.23
3	C	403	BMA	O2-C2-C3	5.46	121.19	110.19
3	A	403	BMA	O2-C2-C3	5.63	121.52	110.19
3	C	403	BMA	C1-O5-C5	7.21	122.75	112.14
3	E	403	BMA	C1-O5-C5	7.48	123.13	112.14
3	B	403	BMA	C1-O5-C5	7.80	123.61	112.14
3	F	403	BMA	C1-O5-C5	8.11	124.06	112.14
3	D	403	BMA	C1-O5-C5	8.53	124.68	112.14
3	A	403	BMA	C1-O5-C5	9.49	126.09	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	403	BMA	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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	335/335 (100%)	-1.00	0 100 100	15, 24, 38, 52	0
1	B	335/335 (100%)	-1.06	0 100 100	13, 21, 37, 58	0
1	C	335/335 (100%)	-1.03	0 100 100	13, 22, 36, 54	0
1	D	335/335 (100%)	-0.99	0 100 100	14, 24, 41, 56	0
1	E	335/335 (100%)	-0.99	0 100 100	15, 25, 42, 56	0
1	F	335/335 (100%)	-1.06	0 100 100	14, 21, 36, 58	0
All	All	2010/2010 (100%)	-1.02	0 100 100	13, 23, 40, 58	0

There are no RSRZ outliers to report.

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	BMA	C	403	11/12	0.71	0.23	21.36	25,30,37,39	0
3	BMA	D	403	11/12	0.83	0.22	19.06	33,34,41,43	0
3	BMA	E	403	11/12	0.86	0.18	14.54	27,34,40,40	0
3	BMA	A	403	11/12	0.81	0.21	12.15	29,34,37,39	0
3	BMA	E	402	12/12	0.84	0.15	10.89	30,36,42,43	0
3	BMA	F	403	11/12	0.77	0.22	10.07	28,30,37,38	0
3	BMA	B	403	11/12	0.82	0.20	9.77	27,32,37,38	0
3	BMA	D	402	12/12	0.95	0.18	8.72	30,33,40,40	0
3	BMA	C	402	12/12	0.92	0.16	8.58	29,35,38,38	0
3	BMA	A	402	12/12	0.95	0.13	7.20	30,34,37,39	0
3	BMA	F	402	12/12	0.93	0.14	4.69	24,31,33,42	0
3	BMA	B	402	12/12	0.96	0.11	2.61	25,29,34,41	0
2	PO4	F	401	5/5	0.99	0.07	-0.11	16,18,20,21	0
2	PO4	D	401	5/5	0.99	0.07	-0.33	17,18,20,21	0
2	PO4	A	401	5/5	0.99	0.07	-0.73	14,18,19,22	0
2	PO4	B	401	5/5	0.99	0.06	-1.25	15,17,18,19	0
2	PO4	E	401	5/5	0.99	0.06	-1.32	18,19,22,23	0
2	PO4	C	401	5/5	0.99	0.06	-2.21	14,14,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.