



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2025 – 02:13 PM EDT

PDB ID : 9MMI / pdb\_00009mmi  
Title : Myo-inositol-1(or 4)-monophosphatase that can perform essential dephosphorylation step to facilitate riboflavin biosynthesis  
Authors : Hoffpauir, Z.A.; Meneely, K.M.; Lamb, A.L.  
Deposited on : 2024-12-20  
Resolution : 1.75 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42



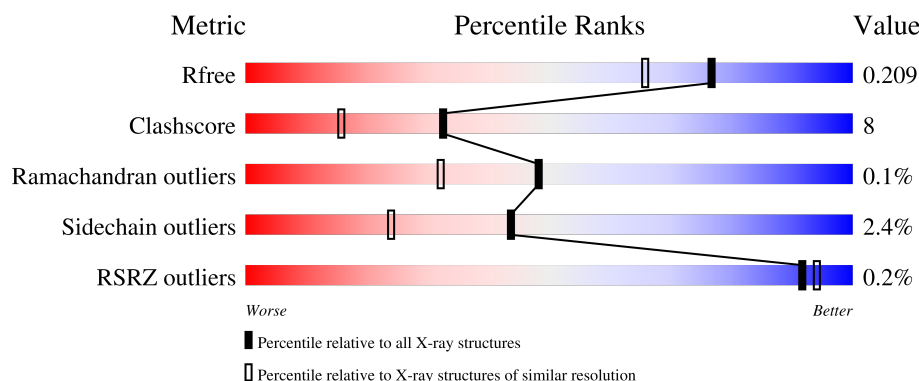
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 1.75 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))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	264	 88% 9% ..
1	B	264	 86% 12% ..
1	C	264	 73% 15% • 12%
1	D	264	 77% 12% • 10%

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	MPD	A	304	-	-	X	-
2	MPD	C	301	-	-	X	-



## 2 Entry composition [i](#)

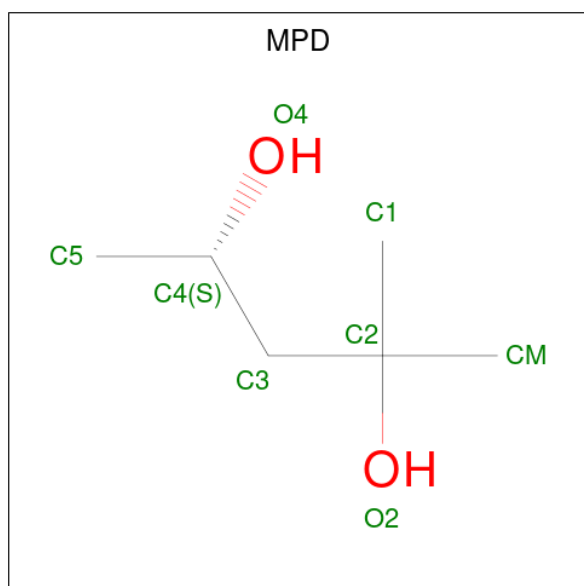
There are 5 unique types of molecules in this entry. The entry contains 16139 atoms, of which 7951 are hydrogens and 0 are deuteriums.

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 Fructose-1,6-bisphosphatase/inositol-1-monophosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	260	Total	C	H	N	O	S	0	1	0
			4108	1333	2060	331	376	8			
1	B	261	Total	C	H	N	O	S	0	1	0
			4119	1336	2066	332	377	8			
1	C	233	Total	C	H	N	O	S	0	0	0
			3657	1199	1837	288	326	7			
1	D	238	Total	C	H	N	O	S	0	0	0
			3717	1217	1862	294	337	7			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	A	1	Total	C	H	O	0	0
			22	6	14	2		

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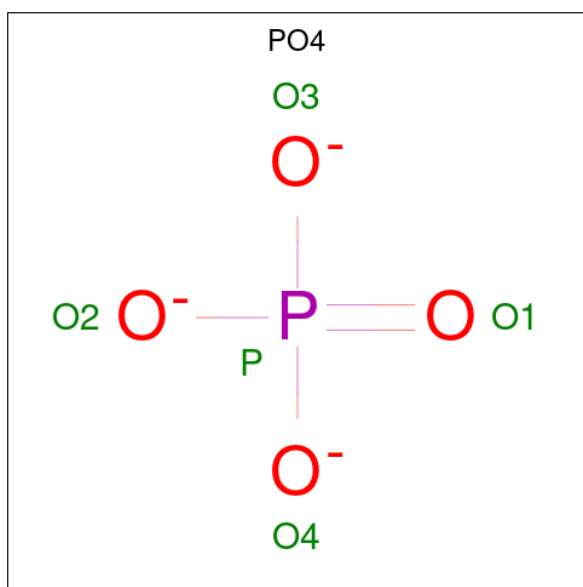
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	B	1	Total	C	H	O	0	0
			22	6	14	2		
2	B	1	Total	C	H	O	0	0
			22	6	14	2		
2	B	1	Total	C	H	O	0	0
			22	6	14	2		
2	B	1	Total	C	H	O	0	0
			22	6	14	2		
2	C	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

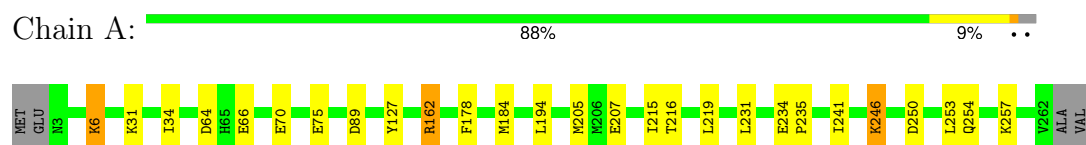
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total	O	0	0
			122	122		
5	B	126	Total	O	0	0
			126	126		
5	C	32	Total	O	0	0
			32	32		
5	D	42	Total	O	0	0
			42	42		



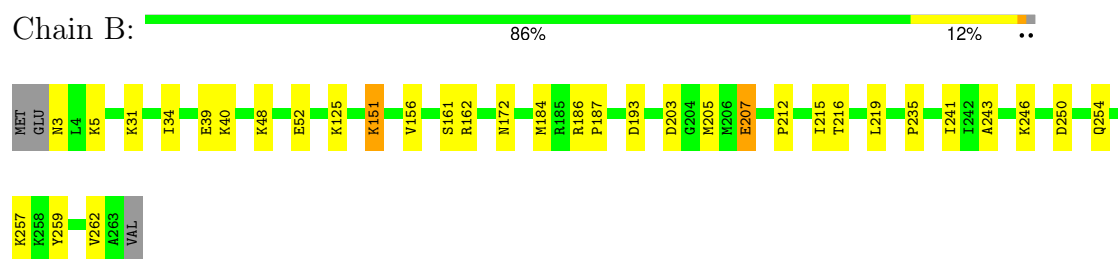
### 3 Residue-property plots

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.

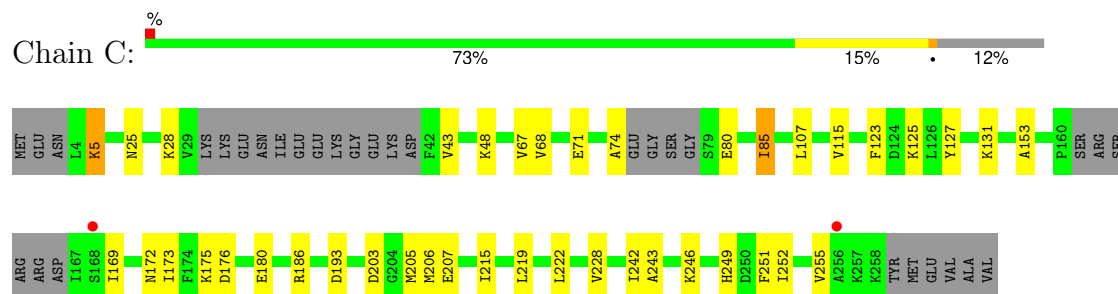
- Molecule 1: Fructose-1,6-bisphosphatase/inositol-1-monophosphatase



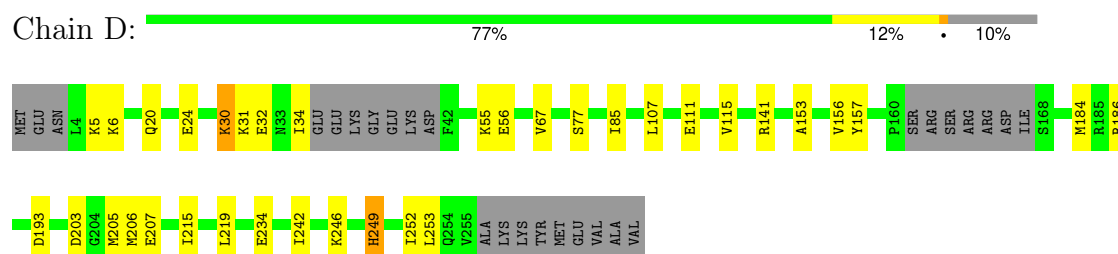
- Molecule 1: Fructose-1,6-bisphosphatase/inositol-1-monophosphatase



- Molecule 1: Fructose-1,6-bisphosphatase/inositol-1-monophosphatase



- Molecule 1: Fructose-1,6-bisphosphatase/inositol-1-monophosphatase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.19Å 72.91Å 119.25Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	37.68 – 1.75 37.68 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.68-1.75) 98.1 (37.68-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.182 , 0.209 0.183 , 0.209	Depositor DCC
$R_{free}$ test set	108778 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.486 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: PO4, MPD, MG

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	0.65	1/2093 (0.0%)	0.77	2/2817 (0.1%)
1	B	0.69	2/2098 (0.1%)	0.80	1/2824 (0.0%)
1	C	0.51	0/1861	0.63	0/2507
1	D	0.52	0/1897	0.66	0/2556
All	All	0.60	3/7949 (0.0%)	0.72	3/10704 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	GLU	CD-OE2	8.25	1.34	1.25
1	B	207	GLU	CD-OE1	-7.13	1.17	1.25
1	A	70	GLU	CD-OE1	-5.08	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	MET	CG-SD-CE	6.56	110.70	100.20
1	A	184	MET	CG-SD-CE	5.47	108.95	100.20
1	A	89	ASP	CB-CG-OD2	-5.18	113.64	118.30



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ARG	Sidechain
1	B	186	ARG	Sidechain
1	D	141	ARG	Sidechain

## 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	2048	2060	2059	30	2
1	B	2053	2066	2064	30	2
1	C	1820	1837	1837	32	0
1	D	1855	1862	1862	23	0
2	A	32	56	56	14	0
2	B	32	56	56	6	0
2	C	8	14	14	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	122	0	0	4	0
5	B	126	0	0	2	0
5	C	32	0	0	1	0
5	D	42	0	0	2	0
All	All	8188	7951	7948	123	2

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 (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:OE2	5:A:401:HOH:O	1.84	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:THR:OG1	2:B:304:MPD:H12	1.78	0.83
2:B:301:MPD:H52	2:B:301:MPD:H11	1.60	0.82
1:A:216:THR:OG1	2:A:304:MPD:H12	1.79	0.82
1:D:32:GLU:OE1	1:D:32:GLU:N	2.16	0.76
2:A:302:MPD:H52	2:A:302:MPD:H11	1.69	0.73
2:A:301:MPD:H13	2:A:301:MPD:H53	1.72	0.71
1:C:43:VAL:HG21	1:C:71:GLU:OE1	1.91	0.70
1:A:219:LEU:HD21	1:A:241[B]:ILE:HD13	1.75	0.69
1:C:74:ALA:O	5:C:401:HOH:O	2.11	0.68
2:C:301:MPD:H52	2:C:301:MPD:HM1	1.75	0.68
1:B:219:LEU:HD21	1:B:241[B]:ILE:HD13	1.74	0.67
1:A:246:LYS:H	1:A:246:LYS:CD	2.08	0.66
1:C:125:LYS:NZ	2:C:301:MPD:H13	2.10	0.65
1:A:246:LYS:H	1:A:246:LYS:CE	2.10	0.65
1:B:215:ILE:HD12	1:B:241[B]:ILE:HD11	1.79	0.63
1:D:215:ILE:HD13	1:D:219:LEU:HD11	1.81	0.62
1:B:219:LEU:HD21	1:B:241[B]:ILE:CD1	2.30	0.61
2:B:301:MPD:H11	2:B:301:MPD:C5	2.29	0.61
1:A:250:ASP:O	1:A:254:GLN:HG2	2.00	0.60
1:B:151:LYS:H	1:B:151:LYS:CE	2.14	0.60
1:A:246:LYS:N	1:A:246:LYS:HD3	2.16	0.60
1:B:156:VAL:HG23	1:B:205:MET:HG3	1.83	0.59
1:A:246:LYS:H	1:A:246:LYS:HD3	1.68	0.58
2:A:302:MPD:H11	2:A:302:MPD:C5	2.34	0.57
1:A:231:LEU:HD13	2:A:304:MPD:C5	2.35	0.57
1:C:80:GLU:OE1	1:C:80:GLU:N	2.22	0.57
1:A:246:LYS:H	1:A:246:LYS:HE2	1.69	0.56
1:A:231:LEU:HD13	2:A:304:MPD:H52	1.87	0.56
1:C:242:ILE:HD12	1:C:252:ILE:HG22	1.86	0.56
1:C:125:LYS:HZ2	2:C:301:MPD:H13	1.71	0.56
1:B:219:LEU:HD21	1:B:241[A]:ILE:HD12	1.88	0.55
1:B:219:LEU:HD21	1:B:241[A]:ILE:CD1	2.37	0.55
1:D:242:ILE:HD12	1:D:252:ILE:HG22	1.88	0.55
1:A:246:LYS:CD	1:A:246:LYS:N	2.69	0.54
1:C:193:ASP:HB3	1:C:205:MET:HE3	1.89	0.54
2:B:302:MPD:O4	2:B:302:MPD:O2	2.26	0.54
1:B:205:MET:HE2	1:B:243:ALA:HB3	1.90	0.54
1:B:151:LYS:H	1:B:151:LYS:HE2	1.73	0.54
1:C:5:LYS:H	1:C:5:LYS:HD2	1.74	0.53
1:B:5:LYS:HG3	5:B:488:HOH:O	2.09	0.53
1:A:219:LEU:HD21	1:A:241[B]:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LYS:HD3	2:B:302:MPD:CM	2.39	0.52
1:A:235:PRO:HB3	2:A:304:MPD:H4	1.91	0.52
1:C:186:ARG:HD3	1:D:184:MET:O	2.09	0.52
1:A:215:ILE:HD12	1:A:241[B]:ILE:HD11	1.91	0.52
1:C:68:VAL:HG22	1:C:74:ALA:HB2	1.91	0.52
1:B:151:LYS:N	1:B:151:LYS:HD3	2.25	0.51
1:B:193:ASP:OD2	1:B:207:GLU:OE2	2.27	0.51
2:C:301:MPD:H52	2:C:301:MPD:CM	2.40	0.51
1:C:85:ILE:HG13	1:C:85:ILE:O	2.10	0.51
1:A:205:MET:CE	1:A:207:GLU:HG3	2.41	0.51
1:C:169:ILE:HD12	1:C:169:ILE:H	1.76	0.51
1:A:6:LYS:NZ	5:A:405:HOH:O	2.45	0.50
1:D:30:LYS:HB3	1:D:32:GLU:OE1	2.11	0.50
1:B:187:PRO:HB2	5:B:402:HOH:O	2.12	0.50
1:B:31:LYS:HA	1:B:34:ILE:HD12	1.94	0.50
1:B:250:ASP:O	1:B:254:GLN:HG2	2.11	0.49
1:A:205:MET:HE2	1:A:207:GLU:HG3	1.94	0.49
1:D:206:MET:O	1:D:206:MET:HG2	2.12	0.49
1:D:215:ILE:O	1:D:219:LEU:HG	2.12	0.49
2:A:302:MPD:C1	5:A:513:HOH:O	2.61	0.48
1:A:66:GLU:OE2	2:A:303:MPD:H52	2.13	0.48
1:C:153:ALA:HA	1:C:203:ASP:OD2	2.13	0.48
2:A:301:MPD:H53	2:A:301:MPD:C1	2.42	0.48
1:C:123:PHE:CE2	2:C:301:MPD:H53	2.49	0.47
1:B:151:LYS:H	1:B:151:LYS:CD	2.27	0.47
1:A:231:LEU:CD1	2:A:304:MPD:H52	2.44	0.47
1:C:172:ASN:HA	1:C:175:LYS:HG2	1.95	0.47
1:B:151:LYS:N	1:B:151:LYS:CD	2.77	0.47
1:C:251:PHE:O	1:C:255:VAL:HG23	2.15	0.47
1:C:228:VAL:HG23	1:C:249:HIS:CD2	2.49	0.47
1:B:3:ASN:CG	1:B:3:ASN:O	2.54	0.46
1:B:257:LYS:HG2	1:B:262:VAL:HG22	1.98	0.46
1:C:127:TYR:OH	2:C:301:MPD:C1	2.63	0.46
1:D:67:VAL:CG1	1:D:85:ILE:CD1	2.93	0.46
1:D:249:HIS:CE1	1:D:253:LEU:HD22	2.50	0.46
1:C:205:MET:HE2	1:C:207:GLU:HG3	1.96	0.46
1:C:175:LYS:HG3	1:C:176:ASP:N	2.30	0.46
1:A:178:PHE:CE2	1:B:161:SER:HA	2.51	0.45
1:C:169:ILE:O	1:C:173:ILE:HG13	2.16	0.45
1:D:5:LYS:HE2	5:D:430:HOH:O	2.15	0.45
1:A:219:LEU:HD21	1:A:241[A]:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LYS:HD2	1:C:5:LYS:N	2.31	0.45
1:D:156:VAL:HG23	1:D:205:MET:HG3	1.98	0.45
1:D:234:GLU:OE1	1:D:234:GLU:HA	2.15	0.45
1:C:215:ILE:HD13	1:C:219:LEU:HD11	1.98	0.45
1:D:31:LYS:O	1:D:34:ILE:HG12	2.17	0.45
1:C:25:ASN:HA	1:C:28:LYS:HD3	1.99	0.45
1:A:253:LEU:O	1:A:257:LYS:HG3	2.17	0.45
1:D:153:ALA:HA	1:D:203:ASP:OD2	2.17	0.44
1:C:215:ILE:O	1:C:219:LEU:HG	2.17	0.44
1:D:193:ASP:OD2	1:D:207:GLU:OE2	2.35	0.44
1:A:235:PRO:HB3	2:A:304:MPD:C5	2.48	0.44
1:D:107:LEU:HB3	1:D:115:VAL:HB	1.99	0.44
1:C:125:LYS:HZ3	2:C:301:MPD:H13	1.81	0.44
1:A:235:PRO:HB3	2:A:304:MPD:C4	2.47	0.44
1:B:48:LYS:O	1:B:52:GLU:HG3	2.19	0.43
1:B:205:MET:HE1	1:B:241[B]:ILE:HG22	1.99	0.43
1:A:219:LEU:HD21	1:A:241[A]:ILE:CD1	2.49	0.43
1:B:156:VAL:O	1:B:205:MET:HA	2.19	0.43
1:B:40:LYS:HG2	1:B:162:ARG:HG3	2.00	0.43
1:A:162:ARG:HA	5:A:484:HOH:O	2.17	0.43
1:B:205:MET:HE1	1:B:241[B]:ILE:CG2	2.49	0.43
1:C:107:LEU:HB3	1:C:115:VAL:HB	2.01	0.42
1:D:157:TYR:CE2	1:D:186:ARG:HD2	2.54	0.42
1:C:222:LEU:HD21	1:C:243:ALA:HB1	2.02	0.42
1:A:31:LYS:HA	1:A:34:ILE:HD12	2.02	0.42
1:C:242:ILE:HD12	1:C:252:ILE:CG2	2.49	0.42
1:B:235:PRO:HB3	2:B:304:MPD:C5	2.50	0.42
1:D:20:GLN:O	1:D:24:GLU:HG3	2.19	0.42
1:A:194:LEU:HD23	1:A:205:MET:SD	2.59	0.41
1:D:242:ILE:HD12	1:D:252:ILE:CG2	2.50	0.41
1:A:127:TYR:OH	2:A:301:MPD:H4	2.20	0.41
1:C:205:MET:CE	1:C:207:GLU:HG3	2.50	0.41
1:C:67:VAL:O	1:C:67:VAL:HG23	2.21	0.41
1:C:206:MET:HG3	1:C:252:ILE:HD13	2.01	0.41
1:D:67:VAL:HG13	1:D:85:ILE:HD11	2.02	0.41
1:B:205:MET:CE	1:B:241[B]:ILE:HG22	2.51	0.41
1:B:172:ASN:HB3	1:B:259:TYR:CZ	2.56	0.41
1:D:6:LYS:NZ	5:D:403:HOH:O	2.42	0.41
1:D:55:LYS:HG2	1:D:67:VAL:CG1	2.51	0.40
1:D:205:MET:HE2	1:D:207:GLU:HG3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLU:OE1	1:B:151:LYS:NZ[2_645]	1.88	0.32
1:A:234:GLU:OE1	1:B:151:LYS:HZ3[2_645]	1.52	0.08

## 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	259/264 (98%)	254 (98%)	5 (2%)	0	100	100
1	B	260/264 (98%)	254 (98%)	6 (2%)	0	100	100
1	C	225/264 (85%)	219 (97%)	6 (3%)	0	100	100
1	D	232/264 (88%)	222 (96%)	9 (4%)	1 (0%)	30	16
All	All	976/1056 (92%)	949 (97%)	26 (3%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	77	SER

### 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	213/215 (99%)	210 (99%)	3 (1%)	62	49
1	B	213/215 (99%)	208 (98%)	5 (2%)	45	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	188/215 (87%)	182 (97%)	6 (3%)	34	14
1	D	192/215 (89%)	187 (97%)	5 (3%)	41	21
All	All	806/860 (94%)	787 (98%)	19 (2%)	44	24

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	64	ASP
1	A	246	LYS
1	B	39	GLU
1	B	151	LYS
1	B	203	ASP
1	B	212	PRO
1	B	246	LYS
1	C	5	LYS
1	C	48	LYS
1	C	85	ILE
1	C	131	LYS
1	C	180	GLU
1	C	246	LYS
1	D	30	LYS
1	D	56	GLU
1	D	111	GLU
1	D	246	LYS
1	D	249	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	249	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	$\# Z  > 2$
2	MPD	C	301	-	7,7,7	0.34	0	9,10,10	0.62	0
4	PO4	B	307	3	4,4,4	1.79	1 (25%)	6,6,6	1.68	2 (33%)
4	PO4	A	307	3	4,4,4	2.11	1 (25%)	6,6,6	1.75	2 (33%)
2	MPD	A	301	-	7,7,7	0.36	0	9,10,10	0.39	0
2	MPD	B	301	-	7,7,7	0.30	0	9,10,10	0.56	0
2	MPD	B	303	-	7,7,7	0.38	0	9,10,10	0.55	0
2	MPD	A	303	-	7,7,7	0.17	0	9,10,10	0.74	0
2	MPD	B	304	-	7,7,7	0.53	0	9,10,10	1.83	2 (22%)
2	MPD	A	304	-	7,7,7	0.63	0	9,10,10	1.53	2 (22%)
2	MPD	A	302	-	7,7,7	0.38	0	9,10,10	0.76	0
2	MPD	B	302	-	7,7,7	0.28	0	9,10,10	0.81	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
2	MPD	C	301	-	-	2/5/5/5	-
2	MPD	A	301	-	-	2/5/5/5	-
2	MPD	B	301	-	-	1/5/5/5	-
2	MPD	B	303	-	-	0/5/5/5	-
2	MPD	A	303	-	-	5/5/5/5	-
2	MPD	B	304	-	-	0/5/5/5	-
2	MPD	A	304	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	A	302	-	-	1/5/5/5	-
2	MPD	B	302	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	307	PO4	P-O4	3.67	1.65	1.54
4	B	307	PO4	P-O4	2.85	1.62	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	307	PO4	O4-P-O2	3.19	117.83	107.91
4	B	307	PO4	O4-P-O2	3.14	117.69	107.91
2	B	304	MPD	C1-C2-C3	-3.08	96.91	110.20
2	B	304	MPD	CM-C2-C3	2.93	122.84	110.20
2	A	304	MPD	C1-C2-C3	-2.84	97.93	110.20
2	A	304	MPD	CM-C2-C3	2.70	121.86	110.20
4	A	307	PO4	O2-P-O1	-2.41	102.44	110.95
4	B	307	PO4	O2-P-O1	-2.20	103.18	110.95

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MPD	C2-C3-C4-C5
2	A	303	MPD	C2-C3-C4-O4
2	A	304	MPD	C2-C3-C4-O4
2	A	304	MPD	C2-C3-C4-C5
2	C	301	MPD	C2-C3-C4-O4
2	C	301	MPD	C2-C3-C4-C5
2	A	302	MPD	O2-C2-C3-C4
2	B	301	MPD	O2-C2-C3-C4
2	A	303	MPD	C1-C2-C3-C4
2	A	303	MPD	C2-C3-C4-C5
2	A	303	MPD	O2-C2-C3-C4
2	A	301	MPD	C2-C3-C4-O4
2	A	303	MPD	CM-C2-C3-C4

There are no ring outliers.

8 monomers are involved in 27 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	MPD	7	0
2	A	301	MPD	3	0
2	B	301	MPD	2	0
2	A	303	MPD	1	0
2	B	304	MPD	2	0
2	A	304	MPD	7	0
2	A	302	MPD	3	0
2	B	302	MPD	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/264 (98%)	-1.39	0 <a href="#">100</a> <a href="#">100</a>	12, 28, 50, 75	1 (0%)
1	B	261/264 (98%)	-1.37	0 <a href="#">100</a> <a href="#">100</a>	12, 28, 51, 77	1 (0%)
1	C	233/264 (88%)	-0.29	2 (0%) <a href="#">81</a> <a href="#">85</a>	30, 55, 84, 98	0
1	D	238/264 (90%)	-0.30	0 <a href="#">100</a> <a href="#">100</a>	30, 56, 88, 107	0
All	All	992/1056 (93%)	-0.86	2 (0%) <a href="#">92</a> <a href="#">94</a>	12, 41, 77, 107	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	168	SER	2.3
1	C	256	ALA	2.2

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MG	C	303	1/1	0.96	0.09	39,39,39,39	0
3	MG	D	302	1/1	0.97	0.10	39,39,39,39	0
2	MPD	A	304	8/8	0.98	0.07	22,45,62,62	0
2	MPD	B	301	8/8	0.98	0.04	30,37,44,53	0
2	MPD	B	302	8/8	0.98	0.06	45,56,68,68	0
2	MPD	B	303	8/8	0.98	0.05	41,53,59,69	0
2	MPD	B	304	8/8	0.98	0.06	24,47,60,68	0
2	MPD	A	302	8/8	0.98	0.04	30,37,43,52	0
3	MG	D	301	1/1	0.98	0.10	46,46,46,46	0
2	MPD	A	303	8/8	0.98	0.06	46,58,70,70	0
2	MPD	A	301	8/8	0.99	0.05	47,56,62,63	0
2	MPD	C	301	8/8	0.99	0.06	67,81,91,91	0
3	MG	C	302	1/1	0.99	0.11	45,45,45,45	0
4	PO4	A	307	5/5	0.99	0.04	23,23,31,32	0
4	PO4	B	307	5/5	0.99	0.05	24,24,31,32	0
3	MG	B	305	1/1	1.00	0.06	15,15,15,15	0
3	MG	B	306	1/1	1.00	0.02	20,20,20,20	0
3	MG	A	305	1/1	1.00	0.07	14,14,14,14	0
3	MG	A	306	1/1	1.00	0.02	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.