



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:44 PM GMT

PDB ID : 4D9C  
Title : PMP bound form of Salmonella typhimurium D-Cysteine desulphydrase obtained after co-crystallization with L-cycloserine  
Authors : Bharath, S.R.; Shveta, B.; Rajesh, K.H.; Savithri, H.S.; Murthy, M.R.N.  
Deposited on : 2012-01-11  
Resolution : 1.97 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

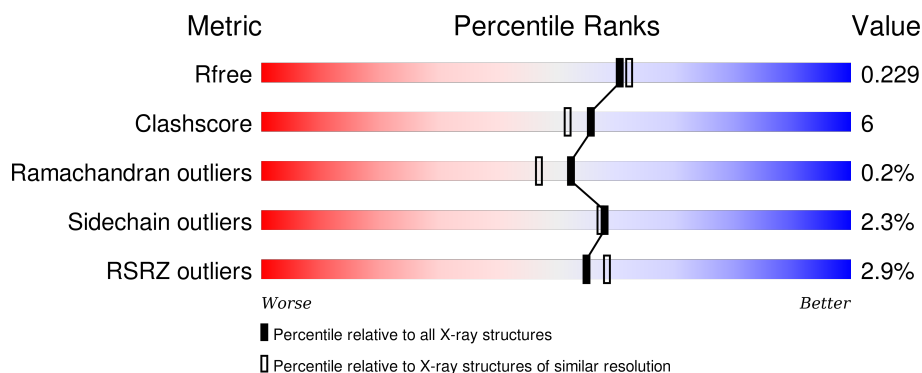
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	342	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>
1	B	342	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	C	342	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 6%</div> </div> </div>
1	D	342	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10545 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 D-Cysteine desulfhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	3	0
			2452	1565	418	460	9			
1	B	319	Total	C	N	O	S	0	3	0
			2386	1519	403	455	9			
1	C	321	Total	C	N	O	S	0	4	0
			2409	1535	411	454	9			
1	D	328	Total	C	N	O	S	0	4	0
			2462	1571	418	464	9			

There are 56 discrepancies between the modelled and reference sequences:

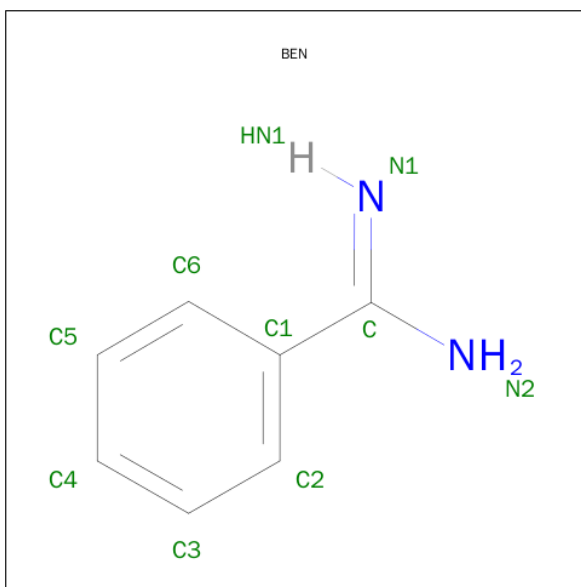
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
A	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
A	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
A	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
A	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
A	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
A	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
B	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
B	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
B	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7

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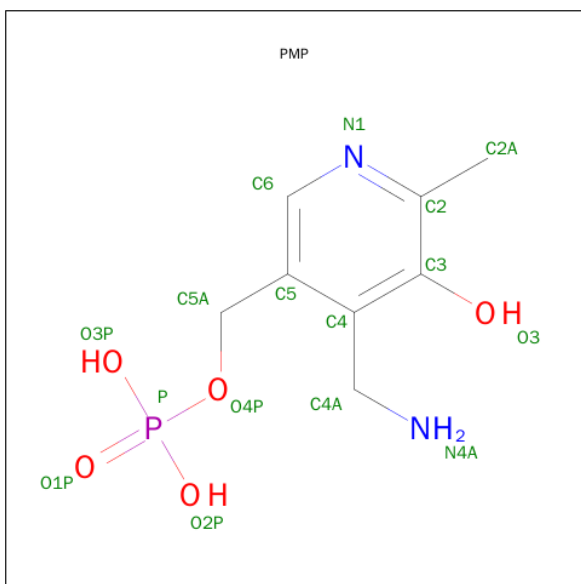
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
B	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
B	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
B	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
B	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
C	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
C	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
C	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
C	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
C	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
C	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
C	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
C	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
C	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7
D	-13	MET	-	EXPRESSION TAG	UNP Q8ZNT7
D	-12	ARG	-	EXPRESSION TAG	UNP Q8ZNT7
D	-11	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
D	-10	SER	-	EXPRESSION TAG	UNP Q8ZNT7
D	-9	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-8	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-7	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-6	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-5	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-4	HIS	-	EXPRESSION TAG	UNP Q8ZNT7
D	-3	GLY	-	EXPRESSION TAG	UNP Q8ZNT7
D	-2	MET	-	EXPRESSION TAG	UNP Q8ZNT7
D	-1	ALA	-	EXPRESSION TAG	UNP Q8ZNT7
D	0	SER	-	EXPRESSION TAG	UNP Q8ZNT7

- Molecule 2 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			9	7	2		
2	C	1	Total	C	N	0	0
			9	7	2		
2	D	1	Total	C	N	0	0
			9	7	2		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula:  $C_8H_{13}N_2O_5P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

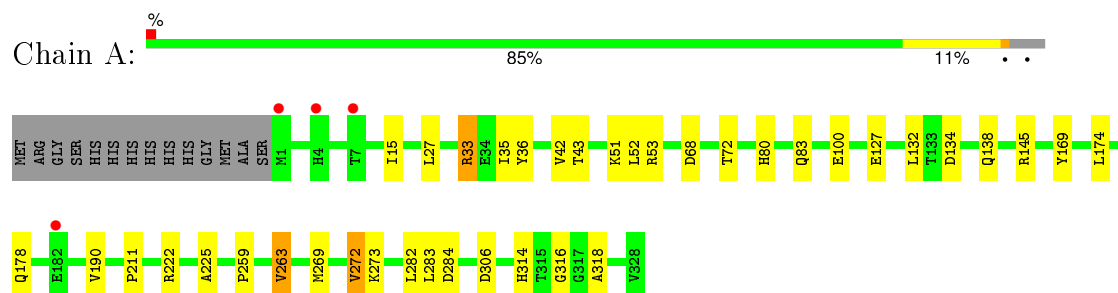
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	234	Total	O	0	0
			234	234		
4	B	152	Total	O	0	0
			152	152		
4	C	142	Total	O	0	0
			142	142		
4	D	217	Total	O	0	0
			217	217		

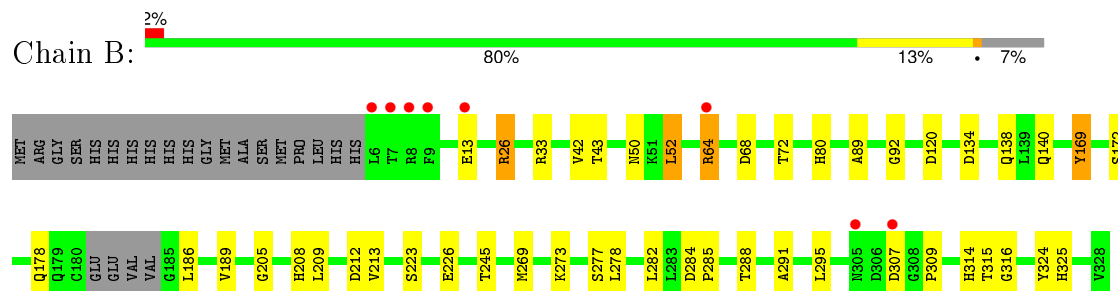
### 3 Residue-property plots [i](#)

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.

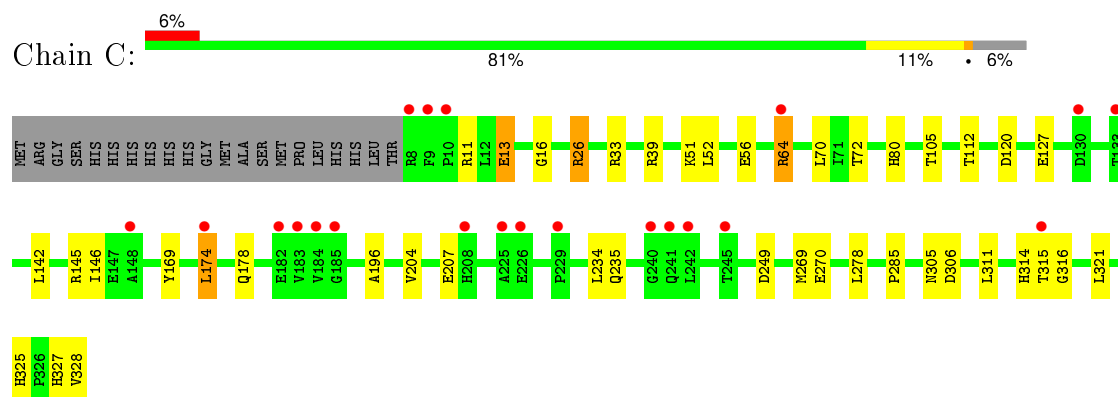
- Molecule 1: D-Cysteine desulphydrase



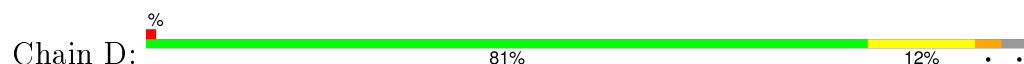
- Molecule 1: D-Cysteine desulphydrase

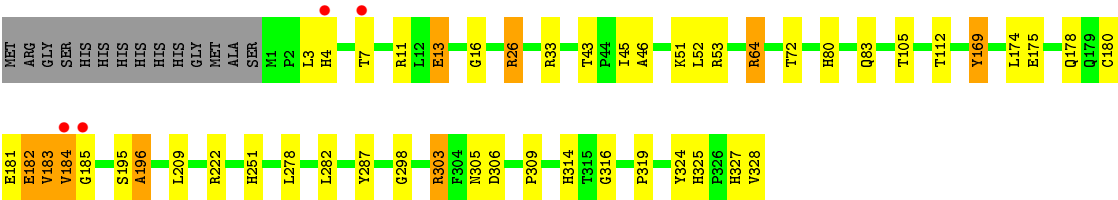


- Molecule 1: D-Cysteine desulphydrase



- Molecule 1: D-Cysteine desulphydrase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.51Å 165.50Å 68.64Å 90.00° 118.89° 90.00°	Depositor
Resolution (Å)	33.71 – 1.97 33.71 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.71-1.97) 99.8 (33.71-1.97)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.85 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.175 , 0.231 0.175 , 0.229	Depositor DCC
$R_{free}$ test set	4572 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.2	EDS
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.019 for h,-k,-h-l 0.022 for -h-l,-k,l 0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 91785 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BEN, PMP

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	1.23	8/2506 (0.3%)	1.01	6/3418 (0.2%)
1	B	1.10	5/2439 (0.2%)	0.99	5/3322 (0.2%)
1	C	1.16	4/2463 (0.2%)	1.07	7/3355 (0.2%)
1	D	1.13	2/2518 (0.1%)	1.04	7/3432 (0.2%)
All	All	1.16	19/9926 (0.2%)	1.03	25/13527 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	GLU	CB-CG	7.98	1.67	1.52
1	A	169	TYR	CD2-CE2	7.38	1.50	1.39
1	A	272	VAL	CB-CG2	7.01	1.67	1.52
1	A	318	ALA	CA-CB	6.34	1.65	1.52
1	D	324	TYR	CD2-CE2	6.05	1.48	1.39
1	B	89	ALA	CA-CB	5.74	1.64	1.52
1	A	225	ALA	CA-CB	5.72	1.64	1.52
1	B	169	TYR	CD2-CE2	5.58	1.47	1.39
1	B	324	TYR	CD2-CE2	5.53	1.47	1.39
1	C	270	GLU	CG-CD	5.45	1.60	1.51
1	B	92	GLY	N-CA	5.28	1.53	1.46
1	C	127	GLU	CB-CG	-5.28	1.42	1.52
1	A	127	GLU	CB-CG	-5.26	1.42	1.52
1	A	222	ARG	CB-CG	-5.18	1.38	1.52
1	A	263	VAL	CB-CG2	5.14	1.63	1.52
1	B	291	ALA	CA-CB	5.13	1.63	1.52
1	C	204	VAL	CB-CG1	5.10	1.63	1.52
1	A	190	VAL	CB-CG1	5.07	1.63	1.52
1	D	175	GLU	CB-CG	-5.04	1.42	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	ARG	NE-CZ-NH1	15.54	128.07	120.30
1	D	26	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	C	26	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	B	26	ARG	NE-CZ-NH2	-13.41	113.60	120.30
1	C	26	ARG	NE-CZ-NH1	12.47	126.53	120.30
1	A	222	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	B	26	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	A	33	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	A	222	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	C	120	ASP	CB-CG-OD1	9.04	126.43	118.30
1	D	222	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	222	ARG	CG-CD-NE	-6.80	97.53	111.80
1	D	169	TYR	CA-CB-CG	-5.91	102.17	113.40
1	B	169	TYR	CA-CB-CG	-5.73	102.51	113.40
1	D	183	VAL	CB-CA-C	-5.67	100.62	111.40
1	C	169	TYR	CA-CB-CG	-5.60	102.77	113.40
1	A	169	TYR	CA-CB-CG	-5.58	102.80	113.40
1	C	70	LEU	CB-CG-CD2	5.55	120.43	111.00
1	B	120	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	68	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	C	26	ARG	CD-NE-CZ	5.32	131.05	123.60
1	B	68	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	183	VAL	N-CA-C	-5.16	97.07	111.00
1	C	311	LEU	CD1-CG-CD2	-5.12	95.16	110.50
1	D	222	ARG	CG-CD-NE	-5.09	101.12	111.80

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	2452	0	2467	25	0
1	B	2386	0	2403	29	0
1	C	2409	0	2428	33	0
1	D	2462	0	2478	37	0
2	A	9	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	9	0	7	0	0
2	D	9	0	7	0	0
3	A	16	0	10	0	0
3	B	16	0	10	1	0
3	C	16	0	11	3	0
3	D	16	0	10	1	0
4	A	234	0	0	4	0
4	B	152	0	0	3	0
4	C	142	0	0	4	0
4	D	217	0	0	4	0
All	All	10545	0	9838	121	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:HG2	1:C:64:ARG:HH11	0.99	1.09
1:D:64:ARG:HG2	1:D:64:ARG:HH11	0.97	1.08
1:D:184:VAL:O	1:D:184:VAL:HG13	1.60	0.98
1:D:64:ARG:HG2	1:D:64:ARG:NH1	1.75	0.97
1:D:105:THR:OG1	1:D:328[A]:VAL:HG12	1.66	0.96
1:C:64:ARG:NH1	1:C:64:ARG:HG2	1.77	0.93
1:C:105:THR:OG1	1:C:328[A]:VAL:HG12	1.68	0.93
1:C:11:ARG:HD2	4:C:615:HOH:O	1.69	0.92
1:D:13:GLU:OE2	1:D:16:GLY:HA2	1.74	0.87
1:C:305:ASN:OD1	1:C:306:ASP:OD1	1.92	0.86
1:B:64:ARG:HH11	1:B:64:ARG:HG2	1.42	0.84
1:D:64:ARG:CG	1:D:64:ARG:HH11	1.89	0.83
1:B:325:HIS:HD2	4:B:631:HOH:O	1.62	0.82
1:C:13:GLU:OE2	1:C:16:GLY:HA2	1.80	0.82
4:A:692:HOH:O	1:C:328[A]:VAL:HG11	1.80	0.80
1:D:184:VAL:O	1:D:184:VAL:CG1	2.30	0.77
4:A:648:HOH:O	1:C:327:HIS:HD2	1.68	0.76
1:D:305[A]:ASN:OD1	1:D:306:ASP:OD1	2.05	0.74
1:A:33:ARG:NH2	4:A:665:HOH:O	2.20	0.74
1:B:314:HIS:HD2	1:B:316:GLY:H	1.36	0.73
1:C:64:ARG:CG	1:C:64:ARG:HH11	1.92	0.67
1:B:314:HIS:CD2	1:B:316:GLY:H	2.14	0.66
1:C:26:ARG:HD3	1:C:278:LEU:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:HIS:HD2	4:D:684:HOH:O	1.78	0.66
1:B:42:VAL:O	1:B:42:VAL:HG12	1.96	0.65
1:D:180:CYS:O	1:D:182:GLU:N	2.30	0.65
1:D:251:HIS:HE1	4:D:685:HOH:O	1.80	0.64
1:A:145:ARG:NH2	1:C:328[A]:VAL:HG21	2.12	0.64
1:B:208:HIS:HE1	1:B:245:THR:O	1.81	0.64
1:D:314:HIS:HD2	1:D:316:GLY:H	1.47	0.63
1:C:39[A]:ARG:NH1	4:C:627:HOH:O	2.31	0.63
1:C:325:HIS:HD2	4:C:616:HOH:O	1.83	0.60
1:B:26:ARG:HD3	1:B:278:LEU:O	2.02	0.60
1:B:169:TYR:CD1	1:B:172[B]:SER:OG	2.51	0.59
1:B:50:ASN:HB2	1:B:169:TYR:CE2	2.37	0.59
1:B:72:THR:OG1	1:B:80:HIS:HE1	1.85	0.58
1:D:287:TYR:CE1	3:D:402:PMP:H4A1	2.38	0.58
1:A:42:VAL:HG22	1:A:42:VAL:O	2.01	0.58
1:A:174:LEU:O	1:A:178:GLN:HG3	2.04	0.57
1:C:314:HIS:HD2	1:C:316:GLY:H	1.50	0.57
1:C:269:MET:SD	1:C:285:PRO:HB3	2.45	0.56
1:B:64:ARG:HG2	1:B:64:ARG:NH1	2.18	0.56
1:B:134:ASP:H	1:B:138:GLN:NE2	2.04	0.56
1:C:315:THR:OG1	3:C:401:PMP:N1	2.29	0.56
1:B:295:LEU:C	1:B:295:LEU:HD23	2.26	0.56
1:B:282:LEU:O	1:B:314:HIS:HE1	1.87	0.56
1:D:181:GLU:O	1:D:182:GLU:CB	2.54	0.56
1:C:145:ARG:HB3	1:C:145:ARG:HH11	1.72	0.54
1:A:282:LEU:O	1:A:314:HIS:HE1	1.89	0.54
1:C:174:LEU:O	1:C:178:GLN:HG3	2.07	0.54
1:A:314:HIS:HD2	1:A:316:GLY:H	1.55	0.54
1:D:13:GLU:OE2	1:D:16:GLY:CA	2.53	0.53
1:A:269:MET:HE3	1:A:273:LYS:HZ1	1.72	0.53
1:C:64:ARG:NH1	1:C:64:ARG:CG	2.60	0.53
1:C:314:HIS:CD2	1:C:316:GLY:H	2.25	0.52
1:A:51:LYS:H	1:A:83:GLN:HE22	1.58	0.52
1:A:72:THR:OG1	1:A:80:HIS:HE1	1.93	0.52
1:A:134:ASP:H	1:A:138:GLN:NE2	2.07	0.52
1:A:132:LEU:HA	1:A:138:GLN:HE22	1.76	0.51
1:D:4:HIS:O	1:D:7:THR:HG22	2.11	0.50
1:D:314:HIS:CD2	1:D:316:GLY:H	2.26	0.50
1:C:145:ARG:HB3	1:C:145:ARG:NH1	2.27	0.50
1:D:26:ARG:HD3	1:D:278:LEU:O	2.11	0.50
1:D:72:THR:OG1	1:D:80:HIS:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:CD1	1:A:53:ARG:HG2	2.42	0.49
1:B:205:GLY:O	1:B:209:LEU:HD12	2.12	0.49
1:B:315:THR:OG1	3:B:401:PMP:N1	2.41	0.48
1:D:306:ASP:O	4:D:713:HOH:O	2.20	0.48
1:D:105:THR:CB	1:D:328[A]:VAL:HG12	2.44	0.48
1:A:145:ARG:HH21	1:C:328[A]:VAL:HG21	1.80	0.47
1:A:134:ASP:H	1:A:138:GLN:HE21	1.61	0.47
1:D:195:SER:O	1:D:196:ALA:HB3	2.13	0.47
1:A:100:GLU:OE2	4:A:596:HOH:O	2.20	0.47
1:B:288:THR:HG21	1:B:314:HIS:CD2	2.48	0.47
1:D:11[B]:ARG:HB3	1:D:11[B]:ARG:HE	1.48	0.46
1:C:51:LYS:HE2	3:C:401:PMP:H4A2	1.97	0.46
1:B:273:LYS:HB2	4:B:593:HOH:O	2.15	0.46
1:A:35[B]:ILE:HD12	1:A:36:TYR:O	2.15	0.46
1:D:282:LEU:O	1:D:314:HIS:HE1	1.97	0.46
1:B:186:LEU:HA	1:B:309:PRO:HB2	1.96	0.46
1:A:52:LEU:HG	1:A:83:GLN:HE21	1.81	0.46
1:B:273:LYS:HE2	1:B:277:SER:HB3	1.98	0.46
1:C:11:ARG:NH2	1:C:56:GLU:OE1	2.50	0.45
1:A:43:THR:OG1	1:A:52:LEU:HD12	2.16	0.45
1:B:223:SER:OG	1:B:226:GLU:HG3	2.17	0.45
1:A:314:HIS:CD2	1:A:316:GLY:H	2.32	0.45
1:C:105:THR:HG1	1:C:328[A]:VAL:HG12	1.74	0.45
1:D:51:LYS:H	1:D:83:GLN:HE22	1.64	0.45
1:C:325:HIS:HE1	1:D:112:THR:OG1	1.99	0.44
1:C:11:ARG:CD	4:C:615:HOH:O	2.45	0.44
1:C:72:THR:OG1	1:C:80:HIS:HE1	2.01	0.44
1:B:42:VAL:CG1	1:B:42:VAL:O	2.65	0.43
1:D:43:THR:OG1	1:D:52:LEU:HD12	2.18	0.43
1:C:285:PRO:HD3	1:C:321:LEU:HD23	2.00	0.43
1:B:134:ASP:H	1:B:138:GLN:HE21	1.66	0.43
1:B:212:ASP:HB2	4:B:604:HOH:O	2.19	0.43
1:C:142:LEU:O	1:C:146:ILE:HG12	2.18	0.43
1:C:112:THR:OG1	1:D:325:HIS:HE1	2.02	0.43
1:D:174:LEU:O	1:D:178:GLN:HG3	2.19	0.43
1:A:269:MET:CE	1:A:273:LYS:NZ	2.82	0.42
1:A:259:PRO:HG2	1:A:263:VAL:HG11	2.01	0.42
1:B:269:MET:SD	1:B:285:PRO:HB3	2.59	0.42
1:C:234:LEU:O	1:C:235:GLN:C	2.58	0.42
1:A:269:MET:HE2	1:A:273:LYS:HZ2	1.85	0.42
1:A:272:VAL:HG22	1:A:283:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:401:PMP:N4A	3:C:401:PMP:O3	2.50	0.41
1:B:189:VAL:HG23	1:B:213:VAL:HG11	2.02	0.41
1:C:13:GLU:OE2	1:C:16:GLY:CA	2.62	0.41
1:D:45:ILE:O	1:D:46:ALA:C	2.58	0.41
1:D:298:GLY:HA2	1:D:303:ARG:HB2	2.02	0.41
1:D:53:ARG:HD2	1:D:169:TYR:CZ	2.56	0.41
1:A:27:LEU:HD23	1:A:35[B]:ILE:HG12	2.01	0.41
1:A:33:ARG:NH2	1:A:306:ASP:O	2.53	0.41
1:B:50:ASN:HB2	1:B:169:TYR:HE2	1.82	0.41
1:B:64:ARG:HH11	1:B:64:ARG:CG	2.21	0.41
1:D:26:ARG:NH2	4:D:668:HOH:O	2.53	0.41
1:D:185:GLY:O	1:D:309:PRO:HD2	2.20	0.41
1:D:3:LEU:HD12	1:D:209:LEU:HD11	2.02	0.40
1:B:43:THR:HB	1:B:52:LEU:HD23	2.02	0.40
1:D:52:LEU:HG	1:D:83:GLN:HE21	1.85	0.40
1:D:327:HIS:CD2	1:D:328[A]:VAL:HG23	2.57	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	329/342 (96%)	319 (97%)	10 (3%)	0	100	100
1	B	318/342 (93%)	310 (98%)	8 (2%)	0	100	100
1	C	322/342 (94%)	306 (95%)	15 (5%)	1 (0%)	46	39
1	D	329/342 (96%)	317 (96%)	10 (3%)	2 (1%)	30	21
All	All	1298/1368 (95%)	1252 (96%)	43 (3%)	3 (0%)	52	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	182	GLU
1	C	196	ALA
1	D	196	ALA

### 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	253/267 (95%)	251 (99%)	2 (1%)	86	88
1	B	249/267 (93%)	241 (97%)	8 (3%)	46	41
1	C	250/267 (94%)	244 (98%)	6 (2%)	57	55
1	D	255/267 (96%)	248 (97%)	7 (3%)	52	50
All	All	1007/1068 (94%)	984 (98%)	23 (2%)	58	57

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	PRO
1	A	284	ASP
1	B	13	GLU
1	B	33	ARG
1	B	52	LEU
1	B	64	ARG
1	B	140	GLN
1	B	178	GLN
1	B	284	ASP
1	B	307	ASP
1	C	13	GLU
1	C	33	ARG
1	C	52	LEU
1	C	64	ARG
1	C	174	LEU
1	C	249	ASP
1	D	13	GLU
1	D	33	ARG
1	D	64	ARG

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Mol	Chain	Res	Type
1	D	183	VAL
1	D	184	VAL
1	D	303	ARG
1	D	319	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	5	HIS
1	A	80	HIS
1	A	83	GLN
1	A	125	GLN
1	A	138	GLN
1	A	208	HIS
1	A	314	HIS
1	B	80	HIS
1	B	83	GLN
1	B	125	GLN
1	B	138	GLN
1	B	140	GLN
1	B	208	HIS
1	B	305	ASN
1	B	314	HIS
1	B	325	HIS
1	C	80	HIS
1	C	83	GLN
1	C	125	GLN
1	C	138	GLN
1	C	314	HIS
1	C	325	HIS
1	C	327	HIS
1	D	80	HIS
1	D	83	GLN
1	D	125	GLN
1	D	138	GLN
1	D	149	GLN
1	D	208	HIS
1	D	251	HIS
1	D	314	HIS
1	D	325	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 ⓘ

7 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	BEN	A	401	-	9,9,9	1.47	1 (11%)	9,11,11	1.47	1 (11%)
3	PMP	A	402	-	16,16,16	1.19	2 (12%)	20,23,23	2.11	6 (30%)
3	PMP	B	401	-	16,16,16	1.16	1 (6%)	20,23,23	1.67	5 (25%)
3	PMP	C	401	-	16,16,16	1.30	3 (18%)	20,23,23	2.02	6 (30%)
2	BEN	C	402	-	9,9,9	1.22	1 (11%)	9,11,11	1.21	1 (11%)
2	BEN	D	401	-	9,9,9	1.36	0	9,11,11	1.28	2 (22%)
3	PMP	D	402	-	16,16,16	1.16	1 (6%)	20,23,23	1.34	3 (15%)

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	BEN	A	401	-	-	0/4/4/4	0/1/1/1
3	PMP	A	402	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PMP	B	401	-	-	0/8/8/8	0/1/1/1
3	PMP	C	401	-	-	0/8/8/8	0/1/1/1
2	BEN	C	402	-	-	0/4/4/4	0/1/1/1
2	BEN	D	401	-	-	0/4/4/4	0/1/1/1
3	PMP	D	402	-	-	0/8/8/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	BEN	C1-C	-2.77	1.42	1.47
3	A	402	PMP	O3-C3	-2.42	1.31	1.37
2	A	401	BEN	C6-C1	2.24	1.43	1.39
3	C	401	PMP	C3-C2	2.31	1.42	1.40
3	A	402	PMP	C2-N1	2.40	1.39	1.34
3	C	401	PMP	C3-C4	2.42	1.43	1.40
3	D	402	PMP	C3-C4	2.47	1.43	1.40
3	C	401	PMP	C6-N1	2.79	1.40	1.34
3	B	401	PMP	C3-C2	3.21	1.43	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	BEN	C5-C6-C1	-2.69	116.96	120.33
3	A	402	PMP	O4P-C5A-C5	-2.56	104.76	108.99
3	C	401	PMP	C5-C6-N1	-2.44	119.62	123.86
3	B	401	PMP	C5-C6-N1	-2.26	119.93	123.86
3	A	402	PMP	C2A-C2-N1	-2.17	113.14	117.95
3	D	402	PMP	C4A-C4-C3	2.17	123.67	120.40
2	D	401	BEN	C3-C2-C1	2.22	123.13	120.33
3	C	401	PMP	O3P-P-O1P	2.29	117.96	110.58
3	C	401	PMP	C4A-C4-C3	2.30	123.87	120.40
2	D	401	BEN	C1-C-N2	2.40	121.94	118.11
3	D	402	PMP	O4P-C5A-C5	2.57	113.25	108.99
3	D	402	PMP	C2A-C2-C3	2.64	124.22	121.04
2	C	402	BEN	C1-C-N2	2.76	122.52	118.11
3	B	401	PMP	C2A-C2-C3	2.94	124.58	121.04
3	B	401	PMP	C6-C5-C4	3.02	120.34	118.09
3	A	402	PMP	C4A-C4-C3	3.06	125.01	120.40
3	B	401	PMP	C4A-C4-C3	3.10	125.07	120.40
3	C	401	PMP	C2A-C2-C3	3.14	124.82	121.04
3	A	402	PMP	O3-C3-C2	3.43	123.63	117.66
3	C	401	PMP	O3-C3-C2	3.50	123.74	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	PMP	O3-C3-C2	3.58	123.89	117.66
3	A	402	PMP	C6-C5-C4	4.21	121.23	118.09
3	A	402	PMP	C2A-C2-C3	4.97	127.03	121.04
3	C	401	PMP	C6-C5-C4	4.99	121.81	118.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	PMP	1	0
3	C	401	PMP	3	0
3	D	402	PMP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<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	328/342 (95%)	-0.23	4 (1%) 81 83	9, 17, 35, 42	0
1	B	319/342 (93%)	0.07	8 (2%) 61 64	12, 24, 41, 52	0
1	C	321/342 (93%)	0.32	21 (6%) 22 25	11, 22, 39, 48	0
1	D	328/342 (95%)	0.03	4 (1%) 81 83	10, 20, 39, 48	0
All	All	1296/1368 (94%)	0.04	37 (2%) 55 58	9, 21, 39, 52	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	THR	4.3
1	C	8	ARG	4.2
1	C	183	VAL	4.2
1	D	184	VAL	4.2
1	B	64	ARG	3.8
1	D	7	THR	3.7
1	C	148	ALA	3.3
1	B	305	ASN	3.2
1	C	185	GLY	3.1
1	D	185	GLY	3.1
1	A	4	HIS	3.1
1	A	1	MET	3.0
1	C	9	PHE	2.8
1	B	9	PHE	2.8
1	C	64	ARG	2.7
1	C	184	VAL	2.6
1	C	182	GLU	2.6
1	C	241	GLN	2.6
1	C	133	THR	2.5
1	C	10	PRO	2.5
1	C	208	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	8	ARG	2.4
1	C	240	GLY	2.4
1	C	174	LEU	2.2
1	C	245	THR	2.2
1	C	315	THR	2.2
1	C	226	GLU	2.1
1	A	7	THR	2.1
1	B	307	ASP	2.1
1	D	4	HIS	2.1
1	C	130	ASP	2.1
1	B	13	GLU	2.1
1	C	229	PRO	2.1
1	A	182	GLU	2.0
1	C	225	ALA	2.0
1	C	242	LEU	2.0
1	B	6	LEU	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 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BEN	C	402	9/9	0.89	0.17	1.35	33,37,38,39	0
3	PMP	C	401	16/16	0.95	0.13	0.26	22,28,35,35	0
3	PMP	B	401	16/16	0.93	0.13	0.22	21,31,33,38	0
2	BEN	A	401	9/9	0.95	0.09	-0.50	12,16,17,18	0
3	PMP	A	402	16/16	0.98	0.10	-0.71	14,17,23,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BEN	D	401	9/9	0.98	0.07	-1.06	9,14,14,16	0
3	PMP	D	402	16/16	0.98	0.09	-2.17	13,19,24,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.