



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 09:38 AM EDT

PDB ID : 4D9B  
Title : Pyridoxamine 5' phosphate (PMP) bound form of Salmonella typhimurium D-Cysteine desulphydrase obtained after co-crystallization with D-cycloserine  
Authors : Bharath, S.R.; Shveta, B.; Rajesh, K.H.; Savithri, H.S.; Murthy, M.R.N.  
Deposited on : 2012-01-11  
Resolution : 1.67 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>.

---

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)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

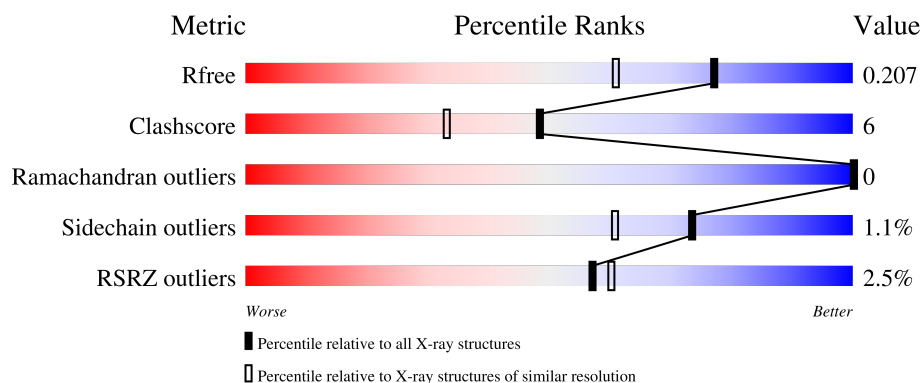
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	342	<div> <div></div> <div>86%</div> <div>10%</div> <div>...</div> </div>
1	B	342	<div> <div>3%</div> <div>86%</div> <div>9%</div> <div>...</div> </div>
1	C	342	<div> <div>5%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	D	342	<div> <div></div> <div>82%</div> <div>13%</div> <div>...</div> </div>

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	EDO	B	403	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10773 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 desulphhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	6	0
			2472	1578	417	468	9			
1	B	328	Total	C	N	O	S	0	1	0
			2427	1549	411	458	9			
1	C	322	Total	C	N	O	S	0	4	0
			2411	1538	407	456	10			
1	D	328	Total	C	N	O	S	3	4	0
			2461	1573	416	463	9			

There are 56 discrepancies between the modelled and reference sequences:

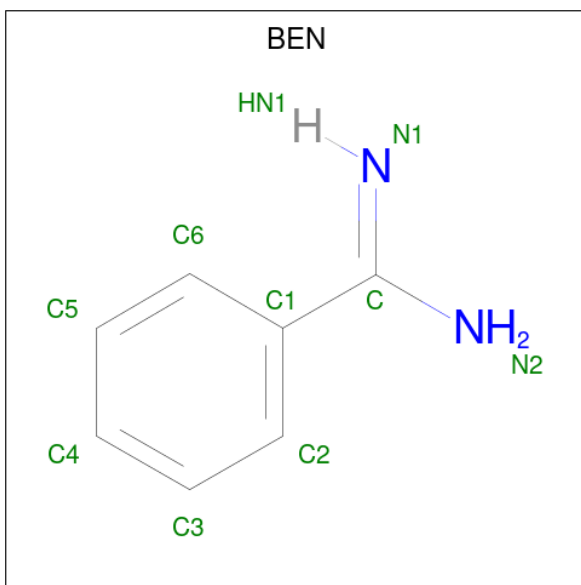
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8ZNT7
A	-12	ARG	-	expression tag	UNP Q8ZNT7
A	-11	GLY	-	expression tag	UNP Q8ZNT7
A	-10	SER	-	expression tag	UNP Q8ZNT7
A	-9	HIS	-	expression tag	UNP Q8ZNT7
A	-8	HIS	-	expression tag	UNP Q8ZNT7
A	-7	HIS	-	expression tag	UNP 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

*Continued on next page...*

*Continued from previous page...*

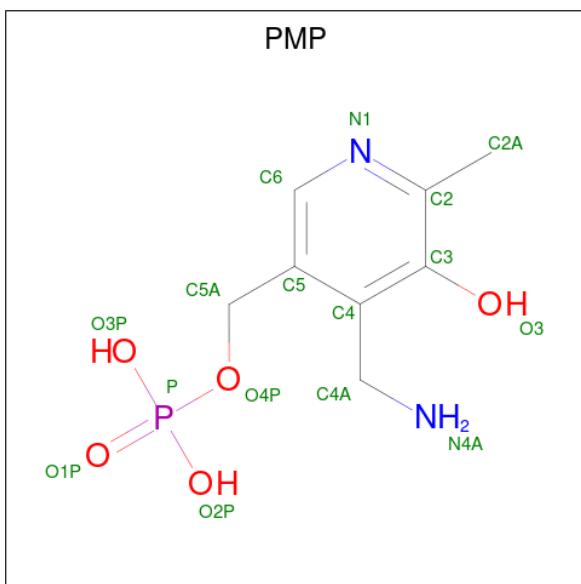
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q8ZNT7
B	-5	HIS	-	expression tag	UNP Q8ZNT7
B	-4	HIS	-	expression tag	UNP Q8ZNT7
B	-3	GLY	-	expression tag	UNP Q8ZNT7
B	-2	MET	-	expression tag	UNP Q8ZNT7
B	-1	ALA	-	expression tag	UNP Q8ZNT7
B	0	SER	-	expression tag	UNP Q8ZNT7
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>).



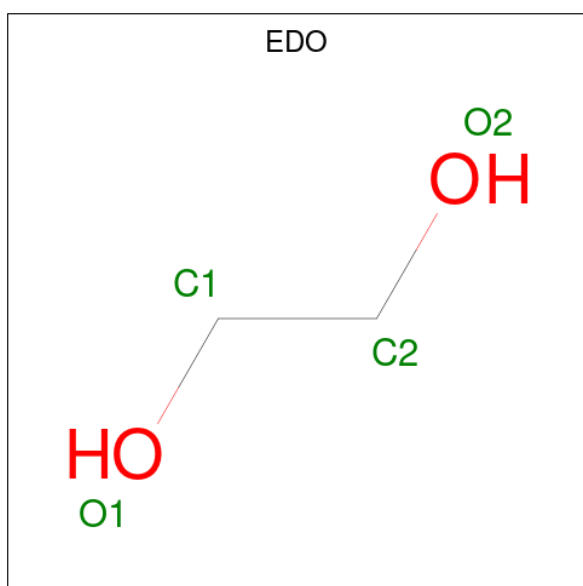
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			9	7	2		
2	C	1	Total	C	N	0	0
			9	7	2		
2	D	1	Total	C	N	0	0
			9	7	2		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P).



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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is water.

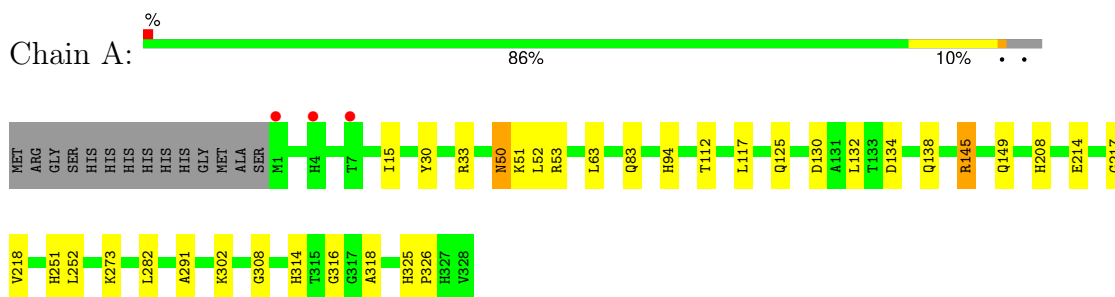
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	256	Total 256	O 256	0	0
5	B	191	Total 191	O 191	0	0
5	C	192	Total 192	O 192	0	0
5	D	248	Total 248	O 248	0	0



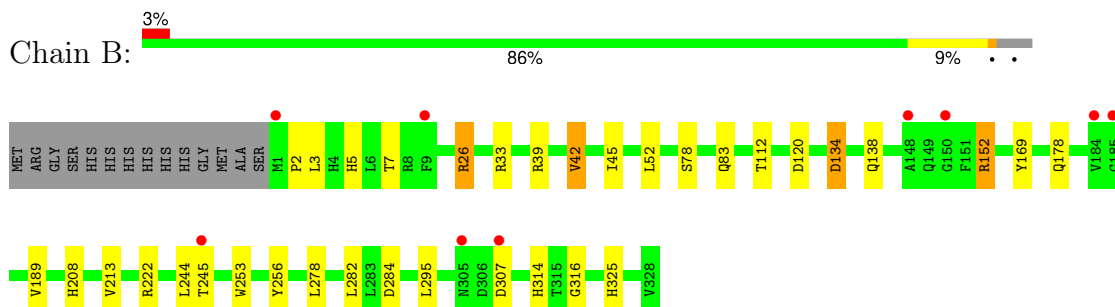
### 3 Residue-property plots

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.

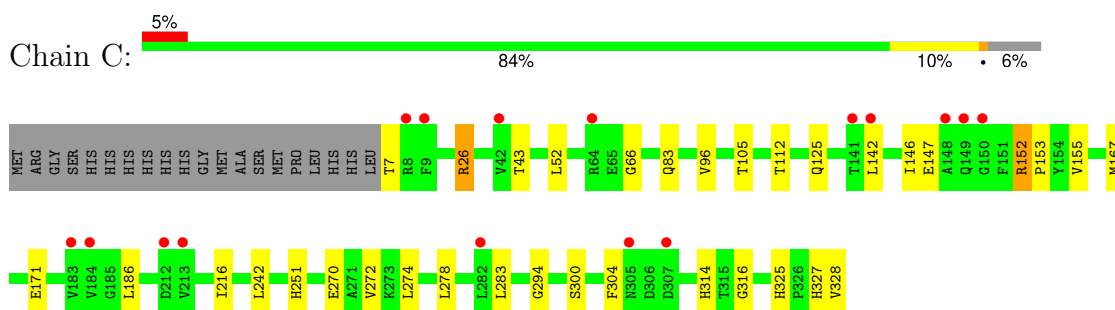
- Molecule 1: D-cysteine desulfhydrase



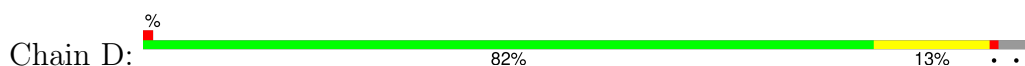
- Molecule 1: D-cysteine desulfhydrase

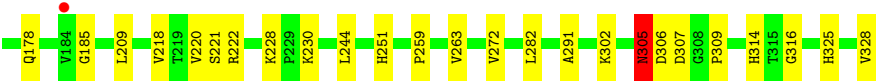
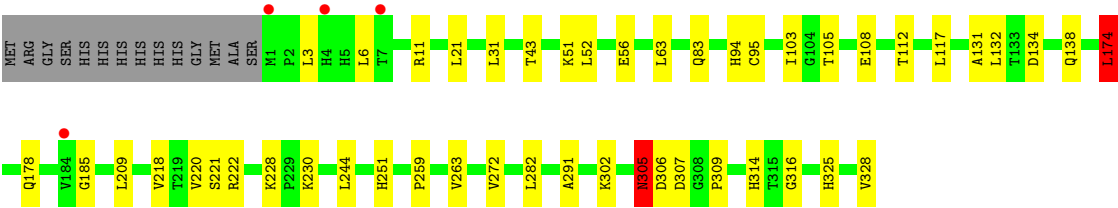


- Molecule 1: D-cysteine desulfhydrase



- Molecule 1: D-cysteine desulfhydrase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.32Å 164.93Å 68.31Å 90.00° 118.97° 90.00°	Depositor
Resolution (Å)	39.91 – 1.67 39.91 – 1.67	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.91-1.67) 97.5 (39.91-1.67)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.171 , 0.206 0.172 , 0.207	Depositor DCC
$R_{free}$ test set	7191 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.019 for h,-k,-h-l 0.023 for -h-l,-k,l 0.020 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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, 0.333 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: BEN, PMP, EDO

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	1.27	2/2539 (0.1%)	1.09	4/3461 (0.1%)
1	B	1.26	5/2477 (0.2%)	1.10	8/3379 (0.2%)
1	C	1.24	2/2465 (0.1%)	1.08	4/3358 (0.1%)
1	D	1.31	8/2517 (0.3%)	1.11	6/3429 (0.2%)
All	All	1.27	17/9998 (0.2%)	1.10	22/13627 (0.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	GLU	CG-CD	5.83	1.60	1.51
1	C	270	GLU	CG-CD	5.78	1.60	1.51
1	D	131	ALA	CA-CB	5.65	1.64	1.52
1	C	294	GLY	N-CA	5.62	1.54	1.46
1	A	318	ALA	CA-CB	5.59	1.64	1.52
1	D	272	VAL	CB-CG2	5.58	1.64	1.52
1	D	220	VAL	CB-CG2	5.48	1.64	1.52
1	B	253	TRP	CG-CD1	5.33	1.44	1.36
1	B	42	VAL	CB-CG2	-5.26	1.41	1.52
1	B	78	SER	CA-CB	5.23	1.60	1.52
1	D	108[A]	GLU	CB-CG	5.21	1.62	1.52
1	D	108[B]	GLU	CB-CG	5.21	1.62	1.52
1	B	45	ILE	C-O	-5.20	1.13	1.23
1	D	228	LYS	CE-NZ	5.20	1.62	1.49
1	D	305	ASN	CB-CG	5.13	1.62	1.51
1	D	302	LYS	CE-NZ	5.03	1.61	1.49
1	B	256	TYR	CE2-CZ	5.01	1.45	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	C	26	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	C	26	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	222	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	B	26	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	D	6	LEU	CA-CB-CG	6.25	129.66	115.30
1	D	31	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	B	134	ASP	CB-CG-OD1	5.86	123.57	118.30
1	D	174	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	169	TYR	CG-CD1-CE1	-5.72	116.72	121.30
1	D	302	LYS	CD-CE-NZ	5.52	124.40	111.70
1	B	169	TYR	CA-CB-CG	-5.39	103.16	113.40
1	A	63	LEU	CB-CG-CD2	5.38	120.14	111.00
1	A	130	ASP	CB-CG-OD1	5.37	123.14	118.30
1	C	186	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	C	274	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	A	273	LYS	CD-CE-NZ	-5.21	99.71	111.70
1	D	63	LEU	CB-CG-CD2	5.17	119.79	111.00
1	D	307	ASP	CB-CA-C	-5.12	100.15	110.40
1	B	307	ASP	CB-CA-C	-5.11	100.17	110.40
1	B	120	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	30	TYR	CB-CG-CD2	-5.05	117.97	121.00

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	2472	0	2486	32	0
1	B	2427	0	2436	21	0
1	C	2411	0	2428	30	0
1	D	2461	0	2482	41	0
2	A	9	0	7	0	0
2	C	9	0	7	1	0
2	D	9	0	7	0	0
3	A	16	0	10	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	10	1	0
3	C	16	0	10	0	0
3	D	16	0	10	0	0
4	A	8	0	12	0	0
4	B	8	0	12	4	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	256	0	0	7	0
5	B	191	0	0	4	0
5	C	192	0	0	6	0
5	D	248	0	0	7	0
All	All	10773	0	9929	118	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 (118) 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:B:3:LEU:HD23	1:B:244:LEU:HD11	1.31	1.12
1:D:105:THR:OG1	1:D:328[A]:VAL:HG12	1.54	1.06
1:C:105:THR:OG1	1:C:328[A]:VAL:HG12	1.64	0.96
1:B:152:ARG:HH11	1:B:152:ARG:HB3	1.34	0.93
1:D:178:GLN:HG3	5:D:748:HOH:O	1.73	0.89
1:C:167[B]:MET:HE1	1:C:242:LEU:HD11	1.56	0.86
1:A:145:ARG:HH12	1:C:328[A]:VAL:HG21	1.40	0.85
1:B:3:LEU:CD2	1:B:244:LEU:HD11	2.06	0.84
1:A:145:ARG:HG2	1:A:145:ARG:HH11	1.44	0.83
1:C:325:HIS:HD2	5:C:622:HOH:O	1.65	0.78
1:D:251:HIS:HE1	5:D:691:HOH:O	1.74	0.70
1:A:325:HIS:HD2	5:A:689:HOH:O	1.74	0.69
1:D:305:ASN:ND2	5:D:732:HOH:O	2.26	0.69
1:C:251:HIS:HE1	5:C:686:HOH:O	1.75	0.69
1:D:305:ASN:OD1	1:D:306:ASP:N	2.26	0.69
1:B:314:HIS:CD2	1:B:316:GLY:H	2.11	0.68
4:B:403:EDO:H22	5:B:684:HOH:O	1.93	0.67
1:A:251:HIS:HE1	5:A:694:HOH:O	1.76	0.67
1:A:208[A]:HIS:HD2	5:A:754:HOH:O	1.77	0.67
1:D:185:GLY:O	1:D:309:PRO:HD2	1.96	0.66
1:B:314:HIS:HD2	1:B:316:GLY:H	1.41	0.66
1:A:314:HIS:HD2	1:A:316:GLY:H	1.44	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:SER:CB	5:C:676:HOH:O	2.42	0.66
1:C:105:THR:HG1	1:C:328[A]:VAL:HG12	1.58	0.65
1:B:208:HIS:HE1	1:B:245:THR:O	1.79	0.65
1:B:325:HIS:HD2	5:B:639:HOH:O	1.79	0.65
1:B:152:ARG:HB3	1:B:152:ARG:NH1	2.11	0.64
1:A:145:ARG:NH1	1:C:328[A]:VAL:HG11	2.13	0.64
1:C:300:SER:HB2	5:C:676:HOH:O	1.98	0.62
1:D:222:ARG:NH2	1:D:230[B]:LYS:HE2	2.15	0.61
1:D:117:LEU:C	1:D:117:LEU:HD23	2.21	0.60
1:B:134:ASP:H	1:B:138:GLN:NE2	1.99	0.60
1:C:66:GLY:O	1:C:152:ARG:HD3	2.02	0.60
1:B:52:LEU:HG	1:B:83:GLN:HE21	1.67	0.59
1:D:134:ASP:H	1:D:138:GLN:NE2	1.99	0.58
1:A:145:ARG:NH1	1:C:328[A]:VAL:HG21	2.15	0.58
1:A:314:HIS:CD2	1:A:316:GLY:H	2.21	0.58
1:C:314:HIS:HD2	1:C:316:GLY:H	1.50	0.57
1:D:314:HIS:HD2	1:D:316:GLY:H	1.53	0.57
1:D:134:ASP:H	1:D:138:GLN:HE21	1.53	0.56
1:D:11:ARG:NH1	1:D:56:GLU:OE1	2.38	0.56
1:D:178:GLN:CG	5:D:748:HOH:O	2.41	0.56
1:A:117:LEU:HD12	5:A:736:HOH:O	2.06	0.56
4:B:403:EDO:H12	1:D:94:HIS:CD2	2.41	0.55
1:D:174:LEU:HD13	1:D:209:LEU:HD11	1.88	0.55
1:A:149:GLN:HE22	1:C:328[A]:VAL:HG22	1.72	0.55
1:D:305:ASN:CG	5:D:732:HOH:O	2.45	0.54
1:D:103:ILE:CD1	1:D:328[B]:VAL:HG21	2.38	0.54
1:C:147:GLU:HG2	1:C:153:PRO:HD2	1.90	0.53
5:A:652:HOH:O	1:C:327:HIS:HD2	1.91	0.53
1:A:302:LYS:HE3	5:A:755:HOH:O	2.08	0.53
1:D:103:ILE:HD11	1:D:328[B]:VAL:HG21	1.91	0.52
1:C:216:ILE:HD13	1:C:304:PHE:CE1	2.45	0.52
1:D:52:LEU:HG	1:D:83:GLN:HE21	1.74	0.52
1:C:300:SER:OG	2:C:401:BEN:H6	2.10	0.52
1:D:314:HIS:CD2	1:D:316:GLY:H	2.28	0.52
1:B:26:ARG:HD3	1:B:278:LEU:O	2.09	0.52
1:D:132:LEU:HA	1:D:138:GLN:HE22	1.75	0.51
1:C:52:LEU:HG	1:C:83:GLN:HE21	1.75	0.51
1:C:105:THR:OG1	1:C:328[A]:VAL:CG1	2.47	0.51
1:A:325:HIS:HE1	1:B:112:THR:OG1	1.93	0.51
1:C:325:HIS:HE1	1:D:112:THR:OG1	1.94	0.51
1:B:282:LEU:O	1:B:314:HIS:HE1	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASP:H	1:A:138:GLN:HE21	1.58	0.50
1:D:51:LYS:H	1:D:83:GLN:HE22	1.58	0.50
1:A:145:ARG:HG2	1:A:145:ARG:NH1	2.20	0.50
1:A:52:LEU:HG	1:A:83:GLN:HE21	1.78	0.49
4:B:403:EDO:H12	1:D:94:HIS:CG	2.47	0.49
1:C:112:THR:OG1	1:D:325:HIS:HE1	1.96	0.49
1:C:314:HIS:CD2	1:C:316:GLY:H	2.29	0.49
1:A:50:ASN:H	1:A:50:ASN:HD22	1.60	0.48
1:C:7:THR:HG23	1:C:167[B]:MET:HE2	1.94	0.48
4:B:403:EDO:H21	5:B:598:HOH:O	2.12	0.48
1:A:134:ASP:H	1:A:138:GLN:NE2	2.12	0.48
1:D:43:THR:OG1	1:D:52:LEU:HD12	2.14	0.48
1:D:282:LEU:O	1:D:314:HIS:HE1	1.97	0.48
1:B:134:ASP:H	1:B:138:GLN:HE21	1.61	0.48
1:D:251:HIS:HD2	5:D:690:HOH:O	1.97	0.48
1:A:51:LYS:H	1:A:83:GLN:HE22	1.61	0.47
1:A:112:THR:OG1	1:B:325:HIS:HE1	1.98	0.47
1:C:96:VAL:HG13	1:C:125:GLN:HG2	1.95	0.46
1:D:105:THR:HG1	1:D:328[A]:VAL:HG12	1.73	0.46
1:D:259:PRO:HG2	1:D:263:VAL:HG11	1.98	0.46
1:B:152:ARG:HH11	1:B:152:ARG:CB	2.18	0.46
1:B:5:HIS:HB2	5:B:676:HOH:O	2.15	0.46
1:A:132:LEU:HA	1:A:138:GLN:HE22	1.80	0.46
1:D:221:SER:C	1:D:222:ARG:HG3	2.36	0.46
1:B:295:LEU:C	1:B:295:LEU:HD23	2.36	0.45
1:C:272:VAL:HG22	1:C:283:LEU:HB2	1.98	0.45
1:D:174:LEU:O	1:D:178:GLN:HG3	2.17	0.45
1:A:282:LEU:O	1:A:314:HIS:HE1	2.00	0.45
1:A:50:ASN:HD22	1:A:50:ASN:N	2.15	0.45
1:C:155:VAL:O	5:C:664:HOH:O	2.21	0.44
1:C:43:THR:OG1	1:C:52:LEU:HD12	2.18	0.44
1:C:142:LEU:O	1:C:146:ILE:HG12	2.18	0.44
3:B:401:PMP:O3	3:B:401:PMP:N4A	2.51	0.44
1:D:105:THR:CB	1:D:328[A]:VAL:HG12	2.45	0.43
1:A:325:HIS:CD2	1:A:326:PRO:HA	2.53	0.43
1:D:21:LEU:HD23	1:D:21:LEU:C	2.39	0.43
1:B:189:VAL:HG23	1:B:213:VAL:HG11	2.01	0.42
1:D:105:THR:HB	1:D:328[B]:VAL:HG22	2.00	0.42
1:A:302:LYS:CE	5:A:755:HOH:O	2.67	0.42
1:A:94:HIS:HD2	5:C:512:HOH:O	2.01	0.42
1:B:39:ARG:O	1:B:42:VAL:HG22	2.20	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:HIS:HE1	1:A:125:GLN:NE2	2.18	0.42
1:A:145:ARG:HH12	1:C:328[A]:VAL:CG2	2.22	0.42
1:D:94:HIS:CD2	1:D:95:CYS:H	2.38	0.42
1:D:230[B]:LYS:HB3	1:D:230[B]:LYS:HE3	1.90	0.42
1:D:51:LYS:HD3	1:D:51:LYS:HA	1.88	0.41
1:A:218:VAL:HG11	1:A:291:ALA:HA	2.01	0.41
1:D:218:VAL:HG11	1:D:291:ALA:HA	2.03	0.41
1:B:2:PRO:O	1:B:244:LEU:HD21	2.20	0.41
1:D:94:HIS:HD2	5:D:538:HOH:O	2.02	0.41
1:C:26:ARG:HD3	1:C:278:LEU:O	2.21	0.40
1:D:3:LEU:HD23	1:D:244:LEU:HD11	2.02	0.40
1:A:33:ARG:HD3	1:A:308:GLY:O	2.22	0.40
1:A:15:ILE:CD1	1:A:53:ARG:HG2	2.52	0.40
1:A:217:GLY:O	1:A:252:LEU:HA	2.22	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	332/342 (97%)	321 (97%)	11 (3%)	0	100	100
1	B	327/342 (96%)	314 (96%)	13 (4%)	0	100	100
1	C	323/342 (94%)	311 (96%)	12 (4%)	0	100	100
1	D	329/342 (96%)	320 (97%)	9 (3%)	0	100	100
All	All	1311/1368 (96%)	1266 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	257/267 (96%)	255 (99%)	2 (1%)	81	72
1	B	250/267 (94%)	245 (98%)	5 (2%)	55	36
1	C	250/267 (94%)	248 (99%)	2 (1%)	81	72
1	D	254/267 (95%)	252 (99%)	2 (1%)	81	72
All	All	1011/1068 (95%)	1000 (99%)	11 (1%)	73	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	145	ARG
1	B	7	THR
1	B	33	ARG
1	B	152	ARG
1	B	178	GLN
1	B	284	ASP
1	C	152	ARG
1	C	171	GLU
1	D	174	LEU
1	D	305	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	50	ASN
1	A	80	HIS
1	A	83	GLN
1	A	94	HIS
1	A	138	GLN
1	A	149	GLN
1	A	251	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	314	HIS
1	A	325	HIS
1	B	80	HIS
1	B	83	GLN
1	B	125	GLN
1	B	138	GLN
1	B	178	GLN
1	B	208	HIS
1	B	301	GLN
1	B	314	HIS
1	B	325	HIS
1	C	80	HIS
1	C	83	GLN
1	C	138	GLN
1	C	251	HIS
1	C	314	HIS
1	C	325	HIS
1	C	327	HIS
1	D	80	HIS
1	D	83	GLN
1	D	94	HIS
1	D	125	GLN
1	D	138	GLN
1	D	140	GLN
1	D	241	GLN
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 monosaccharides in this entry.

## 5.6 Ligand geometry

13 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
4	EDO	A	404	-	3,3,3	0.82	0	2,2,2	1.09	0
2	BEN	D	401	-	9,9,9	2.20	3 (33%)	7,11,11	2.92	5 (71%)
4	EDO	B	403	-	3,3,3	0.24	0	2,2,2	0.28	0
4	EDO	C	403	-	3,3,3	0.74	0	2,2,2	0.91	0
2	BEN	C	401	-	9,9,9	1.20	1 (11%)	7,11,11	2.40	2 (28%)
4	EDO	D	403	-	3,3,3	1.17	0	2,2,2	0.95	0
3	PMP	B	401	-	16,16,16	2.15	5 (31%)	22,23,23	2.64	10 (45%)
3	PMP	D	402	-	16,16,16	1.13	1 (6%)	22,23,23	1.20	2 (9%)
4	EDO	B	402	-	3,3,3	0.49	0	2,2,2	0.98	0
3	PMP	A	402	-	16,16,16	0.97	1 (6%)	22,23,23	2.15	5 (22%)
2	BEN	A	401	-	9,9,9	2.60	4 (44%)	7,11,11	2.07	3 (42%)
4	EDO	A	403	-	3,3,3	0.60	0	2,2,2	0.14	0
3	PMP	C	402	-	16,16,16	2.06	4 (25%)	22,23,23	2.91	9 (40%)

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
4	EDO	A	404	-	-	0/1/1/1	-
2	BEN	D	401	-	-	0/4/4/4	0/1/1/1
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-
2	BEN	C	401	-	-	0/4/4/4	0/1/1/1
4	EDO	D	403	-	-	0/1/1/1	-
3	PMP	B	401	-	-	1/8/8/8	0/1/1/1
3	PMP	D	402	-	-	1/8/8/8	0/1/1/1
4	EDO	B	402	-	-	0/1/1/1	-
3	PMP	A	402	-	-	2/8/8/8	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BEN	A	401	-	-	0/4/4/4	0/1/1/1
4	EDO	A	403	-	-	1/1/1/1	-
3	PMP	C	402	-	-	1/8/8/8	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	PMP	C3-C4	5.86	1.48	1.40
3	B	401	PMP	C3-C2	-4.71	1.36	1.41
2	D	401	BEN	C3-C2	4.62	1.46	1.38
2	A	401	BEN	C6-C1	4.40	1.46	1.39
2	A	401	BEN	C3-C2	3.66	1.45	1.38
3	B	401	PMP	C3-C4	3.63	1.45	1.40
2	A	401	BEN	C4-C3	3.54	1.46	1.38
3	B	401	PMP	C6-N1	3.39	1.41	1.34
3	C	402	PMP	C6-N1	3.27	1.41	1.34
2	A	401	BEN	C5-C6	2.62	1.43	1.38
3	B	401	PMP	O3-C3	-2.53	1.31	1.36
2	D	401	BEN	C4-C3	2.52	1.43	1.38
3	C	402	PMP	C2-N1	2.49	1.38	1.33
2	C	401	BEN	C1-C	-2.37	1.42	1.47
2	D	401	BEN	C1-C	-2.35	1.42	1.47
3	B	401	PMP	P-O4P	2.29	1.67	1.60
3	A	402	PMP	O3-C3	-2.29	1.31	1.36
3	C	402	PMP	P-O3P	-2.14	1.46	1.54
3	D	402	PMP	P-O2P	-2.10	1.47	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	PMP	C6-C5-C4	8.94	124.82	118.06
3	B	401	PMP	C6-C5-C4	7.32	123.60	118.06
3	A	402	PMP	C6-C5-C4	6.99	123.35	118.06
2	C	401	BEN	C1-C-N2	5.52	126.39	118.01
3	B	401	PMP	O3-C3-C2	4.84	127.61	117.58
3	C	402	PMP	C5-C6-N1	-4.59	116.36	123.83
2	D	401	BEN	C5-C6-C1	-4.50	115.94	120.36
3	C	402	PMP	C5A-C5-C6	-4.49	112.04	119.36
3	C	402	PMP	O3-C3-C2	4.25	126.39	117.58
2	D	401	BEN	C4-C5-C6	4.22	125.45	120.24
3	B	401	PMP	C5-C6-N1	-3.90	117.48	123.83
3	A	402	PMP	C3-C4-C5	-3.73	115.34	118.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	PMP	C5-C6-N1	-3.71	117.79	123.83
3	B	401	PMP	C3-C2-N1	3.60	125.50	120.96
2	A	401	BEN	C5-C6-C1	-3.36	117.06	120.36
3	B	401	PMP	O4P-C5A-C5	-2.91	103.91	109.36
3	C	402	PMP	C4-C3-C2	-2.85	115.60	119.91
2	D	401	BEN	C6-C1-C2	2.81	122.14	118.57
3	D	402	PMP	C4A-C4-C3	2.68	124.76	120.22
2	D	401	BEN	C4-C3-C2	-2.43	117.24	120.24
3	C	402	PMP	O3P-P-O2P	2.42	116.88	107.80
3	B	401	PMP	O3P-P-O2P	2.38	116.73	107.80
2	D	401	BEN	C1-C-N2	2.34	121.57	118.01
2	A	401	BEN	C4-C5-C6	2.33	123.11	120.24
3	C	402	PMP	C3-C2-N1	2.32	123.89	120.96
3	C	402	PMP	C4A-C4-C3	2.29	124.11	120.22
3	A	402	PMP	C5A-C5-C6	-2.29	115.63	119.36
3	B	401	PMP	O2P-P-O4P	2.25	112.55	106.67
3	D	402	PMP	C4A-C4-C5	-2.25	115.75	120.27
3	B	401	PMP	C4-C3-C2	-2.22	116.56	119.91
3	A	402	PMP	C6-N1-C2	2.19	123.17	119.20
2	A	401	BEN	C4-C3-C2	-2.10	117.65	120.24
2	C	401	BEN	C5-C6-C1	2.07	122.40	120.36
3	B	401	PMP	C2A-C2-N1	-2.06	113.76	117.64
3	C	402	PMP	C2A-C2-N1	-2.04	113.81	117.64
3	B	401	PMP	C3-C4-C5	-2.02	116.90	118.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PMP	C3-C4-C4A-N4A
3	B	401	PMP	C3-C4-C4A-N4A
3	C	402	PMP	C3-C4-C4A-N4A
3	D	402	PMP	C3-C4-C4A-N4A
3	A	402	PMP	C5-C4-C4A-N4A
4	A	403	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	EDO	4	0
2	C	401	BEN	1	0
3	B	401	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%)	-0.40	3 (0%) 84 87	11, 16, 33, 44	0
1	B	328/342 (95%)	-0.12	9 (2%) 54 57	13, 20, 42, 52	0
1	C	322/342 (94%)	0.15	16 (4%) 28 30	13, 23, 40, 52	0
1	D	328/342 (95%)	-0.32	4 (1%) 79 82	11, 17, 34, 42	1 (0%)
All	All	1306/1368 (95%)	-0.18	32 (2%) 57 60	11, 19, 38, 52	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	VAL	5.6
1	B	305	ASN	4.3
1	D	7	THR	4.3
1	C	183	VAL	4.0
1	C	8	ARG	3.9
1	C	142	LEU	3.7
1	A	1	MET	3.6
1	A	4	HIS	3.0
1	C	148	ALA	3.0
1	C	149	GLN	2.9
1	B	1	MET	2.8
1	B	148	ALA	2.7
1	C	150	GLY	2.7
1	A	7	THR	2.7
1	C	307	ASP	2.6
1	B	245	THR	2.6
1	D	184	VAL	2.6
1	D	1	MET	2.6
1	B	9	PHE	2.5
1	C	282	LEU	2.5
1	B	307	ASP	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	184	VAL	2.5
1	B	185	GLY	2.5
1	C	212	ASP	2.4
1	C	9	PHE	2.4
1	B	150	GLY	2.4
1	C	141	THR	2.4
1	C	42	VAL	2.2
1	D	4	HIS	2.2
1	C	64	ARG	2.1
1	C	305	ASN	2.1
1	C	213	VAL	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<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(Å <sup>2</sup> )	Q<0.9
4	EDO	D	403	4/4	0.82	0.12	23,27,32,32	0
4	EDO	B	402	4/4	0.89	0.12	29,33,35,35	0
4	EDO	B	403	4/4	0.91	0.12	24,30,30,33	0
4	EDO	A	403	4/4	0.91	0.17	36,37,40,41	0
4	EDO	A	404	4/4	0.92	0.10	25,28,30,31	0
4	EDO	C	403	4/4	0.93	0.07	28,28,30,30	0
2	BEN	C	401	9/9	0.93	0.14	27,31,34,36	0
2	BEN	A	401	9/9	0.95	0.07	14,15,17,18	0
2	BEN	D	401	9/9	0.96	0.06	13,14,16,17	0
3	PMP	C	402	16/16	0.97	0.10	14,18,22,23	0
3	PMP	B	401	16/16	0.98	0.08	11,15,20,22	0
3	PMP	A	402	16/16	0.98	0.08	11,13,17,22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PMP	D	402	16/16	0.99	0.09	11,13,16,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.