



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:48 AM GMT

PDB ID : 3Q1O  
Title : Crystal structure of geranyltransferase from helicobacter pylori complexed with magnesium and isoprenyl diphosphate  
Authors : Patskovsky, Y.; Toro, R.; Rutter, M.; Sauder, J.M.; Burley, S.K.; Poulter, C.D.; Gerlt, J.A.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2010-12-17  
Resolution : 2.40 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

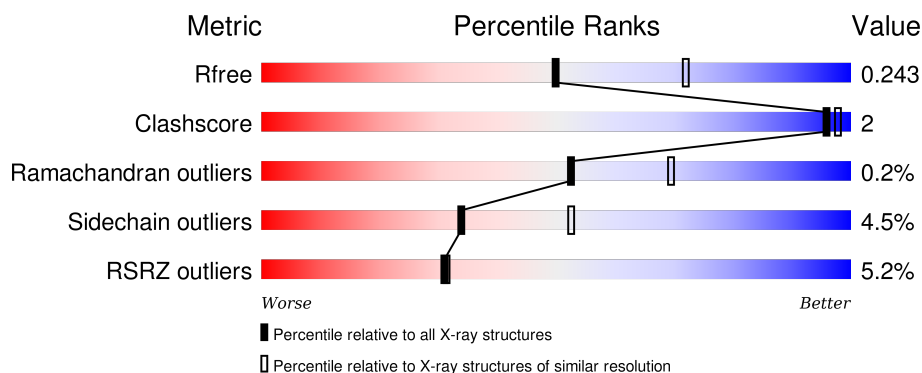
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	310	<div> <div>2%</div> <div>90%</div> <div>8% •</div> </div>
1	B	310	<div> <div>4%</div> <div>90%</div> <div>8% •</div> </div>
1	C	310	<div> <div>3%</div> <div>91%</div> <div>5% • •</div> </div>
1	D	310	<div> <div>12%</div> <div>88%</div> <div>8% •</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10049 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 Geranyltranstransferase (IspA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	5	0
			2445	1573	403	457	12			
1	B	303	Total	C	N	O	S	0	2	0
			2428	1559	401	457	11			
1	C	301	Total	C	N	O	S	0	2	0
			2416	1552	398	455	11			
1	D	299	Total	C	N	O	S	0	0	0
			2384	1533	391	449	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP O25583
A	-7	ALA	-	EXPRESSION TAG	UNP O25583
A	-6	HIS	-	EXPRESSION TAG	UNP O25583
A	-5	HIS	-	EXPRESSION TAG	UNP O25583
A	-4	HIS	-	EXPRESSION TAG	UNP O25583
A	-3	HIS	-	EXPRESSION TAG	UNP O25583
A	-2	HIS	-	EXPRESSION TAG	UNP O25583
A	-1	HIS	-	EXPRESSION TAG	UNP O25583
A	0	SER	-	EXPRESSION TAG	UNP O25583
A	1	LEU	-	EXPRESSION TAG	UNP O25583
B	-8	MET	-	EXPRESSION TAG	UNP O25583
B	-7	ALA	-	EXPRESSION TAG	UNP O25583
B	-6	HIS	-	EXPRESSION TAG	UNP O25583
B	-5	HIS	-	EXPRESSION TAG	UNP O25583
B	-4	HIS	-	EXPRESSION TAG	UNP O25583
B	-3	HIS	-	EXPRESSION TAG	UNP O25583
B	-2	HIS	-	EXPRESSION TAG	UNP O25583
B	-1	HIS	-	EXPRESSION TAG	UNP O25583
B	0	SER	-	EXPRESSION TAG	UNP O25583
B	1	LEU	-	EXPRESSION TAG	UNP O25583
C	-8	MET	-	EXPRESSION TAG	UNP O25583

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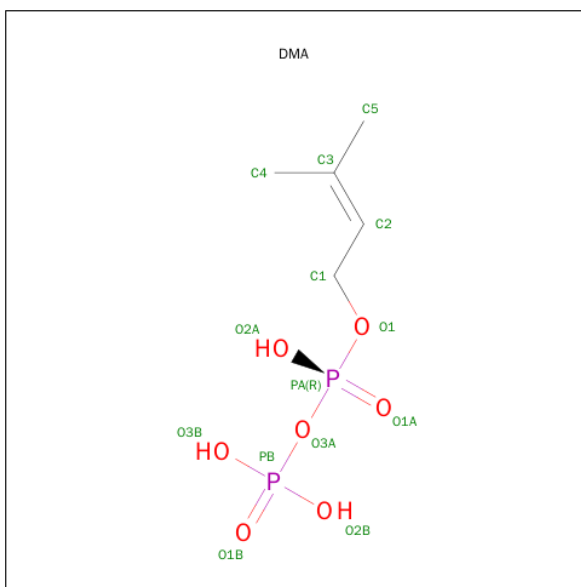
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	EXPRESSION TAG	UNP O25583
C	-6	HIS	-	EXPRESSION TAG	UNP O25583
C	-5	HIS	-	EXPRESSION TAG	UNP O25583
C	-4	HIS	-	EXPRESSION TAG	UNP O25583
C	-3	HIS	-	EXPRESSION TAG	UNP O25583
C	-2	HIS	-	EXPRESSION TAG	UNP O25583
C	-1	HIS	-	EXPRESSION TAG	UNP O25583
C	0	SER	-	EXPRESSION TAG	UNP O25583
C	1	LEU	-	EXPRESSION TAG	UNP O25583
D	-8	MET	-	EXPRESSION TAG	UNP O25583
D	-7	ALA	-	EXPRESSION TAG	UNP O25583
D	-6	HIS	-	EXPRESSION TAG	UNP O25583
D	-5	HIS	-	EXPRESSION TAG	UNP O25583
D	-4	HIS	-	EXPRESSION TAG	UNP O25583
D	-3	HIS	-	EXPRESSION TAG	UNP O25583
D	-2	HIS	-	EXPRESSION TAG	UNP O25583
D	-1	HIS	-	EXPRESSION TAG	UNP O25583
D	0	SER	-	EXPRESSION TAG	UNP O25583
D	1	LEU	-	EXPRESSION TAG	UNP O25583

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is DIMETHYLALLYL DIPHOSPHATE (three-letter code: DMA) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	7	2		
3	A	1	Total	C	O	P	0	0
			14	5	7	2		
3	B	1	Total	C	O	P	0	0
			14	5	7	2		
3	B	1	Total	C	O	P	0	0
			14	5	7	2		
3	C	1	Total	C	O	P	0	0
			14	5	7	2		
3	C	1	Total	C	O	P	0	0
			14	5	7	2		
3	D	1	Total	C	O	P	0	0
			14	5	7	2		
3	D	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



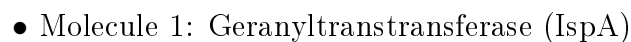
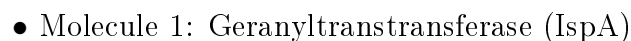
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		
5	B	57	Total	O	0	0
			57	57		
5	C	63	Total	O	0	0
			63	63		
5	D	24	Total	O	0	0
			24	24		



- Molecule 1: Geranyltranstransferase (IspA)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.87Å 191.87Å 127.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 49.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.40) 97.8 (49.08-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.214 , 0.243 0.214 , 0.243	Depositor DCC
$R_{free}$ test set	2778 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 102864 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMA, MG, SO4

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	0.38	0/2508	0.53	0/3390
1	B	0.38	0/2482	0.53	0/3358
1	C	0.37	0/2466	0.52	0/3338
1	D	0.38	0/2433	0.54	0/3293
All	All	0.38	0/9889	0.53	0/13379

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	2445	0	2449	8	0
1	B	2428	0	2414	7	0
1	C	2416	0	2403	6	0
1	D	2384	0	2373	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	18	0	0
3	C	28	0	18	2	0
3	D	28	0	18	1	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
4	C	15	0	0	0	0
5	A	80	0	0	0	0
5	B	57	0	0	0	0
5	C	63	0	0	0	0
5	D	24	0	0	1	0
All	All	10049	0	9711	30	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 2.

All (30) 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:250[A]:LYS:HG2	1:A:251[A]:ASN:H	1.57	0.68
1:B:183:HIS:HD2	1:B:253:PHE:CE2	2.17	0.62
1:A:257:LEU:HB3	1:A:261:ARG:HB3	1.89	0.55
1:A:89:LEU:HD13	1:A:103:ARG:HD3	1.91	0.53
1:B:246:LEU:HB2	1:B:249:ALA:HB2	1.90	0.52
1:B:183:HIS:HD2	1:B:253:PHE:HE2	1.57	0.52
1:B:61:LEU:HB3	1:B:204:ILE:HD12	1.92	0.52
1:C:140:SER:HB2	1:D:140:SER:HB3	1.90	0.51
1:D:242:LYS:HB2	5:D:312:HOH:O	2.10	0.51
1:D:179:LEU:HD11	1:D:251:ASN:HB3	1.94	0.50
1:C:251[A]:ASN:N	1:C:251[A]:ASN:OD1	2.46	0.48
1:D:89:LEU:HD23	3:D:501:DMA:H42	1.96	0.47
1:D:195:LEU:HB3	1:D:213:LEU:HD22	1.96	0.47
1:C:186:LYS:HG2	3:C:501:DMA:H2	1.95	0.47
1:A:188:ALA:HB1	1:A:218:LEU:HA	1.98	0.46
1:A:58:LEU:HD21	1:A:74:TYR:CG	2.51	0.46
1:D:53:LEU:HD22	1:D:195:LEU:HD21	1.98	0.45
1:B:58:LEU:HD21	1:B:74:TYR:CG	2.52	0.45
1:B:250:LYS:O	1:B:255:ASN:ND2	2.50	0.42
1:C:103:ARG:HG2	1:C:104:ARG:HG3	2.00	0.42
1:D:47:LYS:HB3	1:D:47:LYS:HE2	1.80	0.42
1:D:6:LEU:HD13	1:D:289:GLU:HG2	2.01	0.41
1:A:186:LYS:HG2	3:A:501:DMA:H2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250[A]:LYS:HG2	1:A:251[A]:ASN:N	2.32	0.41
1:B:57:VAL:HA	1:B:287:LEU:HD13	2.01	0.41
1:C:188:ALA:HB1	1:C:218:LEU:HA	2.03	0.41
1:D:58:LEU:C	1:D:60:ALA:H	2.23	0.41
3:C:500:DMA:H53	3:C:501:DMA:C2	2.51	0.41
1:C:140:SER:HB2	1:D:140:SER:CB	2.51	0.41
1:A:166:ASP:HA	1:A:182:LEU:HD11	2.04	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	306/310 (99%)	297 (97%)	9 (3%)	0	100	100
1	B	303/310 (98%)	293 (97%)	10 (3%)	0	100	100
1	C	301/310 (97%)	292 (97%)	9 (3%)	0	100	100
1	D	297/310 (96%)	283 (95%)	12 (4%)	2 (1%)	26	38
All	All	1207/1240 (97%)	1165 (96%)	40 (3%)	2 (0%)	52	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	ASN
1	D	59	CYS

### 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	271/272 (100%)	260 (96%)	11 (4%)	37	57
1	B	268/272 (98%)	255 (95%)	13 (5%)	31	48
1	C	267/272 (98%)	252 (94%)	15 (6%)	26	41
1	D	263/272 (97%)	253 (96%)	10 (4%)	40	60
All	All	1069/1088 (98%)	1020 (95%)	49 (5%)	34	51

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	25	LEU
1	A	48	ARG
1	A	62	VAL
1	A	66	ASP
1	A	70	GLN
1	A	87	TYR
1	A	97	MET
1	A	126	ASN
1	A	183	HIS
1	A	270	LYS
1	B	-1	HIS
1	B	36	LYS
1	B	41	MET
1	B	48	ARG
1	B	80	SER
1	B	87	TYR
1	B	126	ASN
1	B	189	LYS
1	B	220	MET
1	B	222	LEU
1	B	223	CYS
1	B	277	LEU
1	B	300	LYS
1	C	25	LEU
1	C	41	MET
1	C	48	ARG
1	C	62	VAL
1	C	84	LEU
1	C	87	TYR

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Mol	Chain	Res	Type
1	C	97	MET
1	C	126	ASN
1	C	140	SER
1	C	172	THR
1	C	183	HIS
1	C	192	SER
1	C	250	LYS
1	C	251[A]	ASN
1	C	251[B]	ASN
1	D	27	LEU
1	D	48	ARG
1	D	66	ASP
1	D	70	GLN
1	D	87	TYR
1	D	126	ASN
1	D	177	GLU
1	D	246	LEU
1	D	261	ARG
1	D	272	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	126	ASN
1	B	44	ASN
1	B	126	ASN
1	B	153	ASN
1	B	183	HIS
1	C	44	ASN
1	C	126	ASN
1	D	44	ASN
1	D	69	ASN
1	D	126	ASN
1	D	214	GLN
1	D	235	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	$\# Z  > 2$
4	SO4	A	302	-	4,4,4	0.19	0	6,6,6	0.17	0
4	SO4	A	303	-	4,4,4	0.21	0	6,6,6	0.13	0
4	SO4	A	304	-	4,4,4	0.23	0	6,6,6	0.15	0
3	DMA	A	500	-	11,13,13	0.57	0	16,19,19	1.48	3 (18%)
3	DMA	A	501	2	11,13,13	0.58	0	16,19,19	1.50	2 (12%)
4	SO4	B	302	-	4,4,4	0.21	0	6,6,6	0.10	0
3	DMA	B	500	-	11,13,13	0.54	0	16,19,19	1.42	2 (12%)
3	DMA	B	501	2	11,13,13	0.60	0	16,19,19	1.54	2 (12%)
4	SO4	C	302	-	4,4,4	0.30	0	6,6,6	0.19	0
4	SO4	C	303	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	C	304	-	4,4,4	0.20	0	6,6,6	0.06	0
3	DMA	C	500	-	11,13,13	0.55	0	16,19,19	1.50	2 (12%)
3	DMA	C	501	2	11,13,13	0.55	0	16,19,19	1.64	3 (18%)
3	DMA	D	500	-	11,13,13	0.60	0	16,19,19	1.24	3 (18%)
3	DMA	D	501	2	11,13,13	0.60	0	16,19,19	1.45	2 (12%)

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	SO4	A	302	-	-	0/0/0/0	0/0/0/0
4	SO4	A	303	-	-	0/0/0/0	0/0/0/0
4	SO4	A	304	-	-	0/0/0/0	0/0/0/0
3	DMA	A	500	-	-	0/13/13/13	0/0/0/0
3	DMA	A	501	2	-	0/13/13/13	0/0/0/0
4	SO4	B	302	-	-	0/0/0/0	0/0/0/0
3	DMA	B	500	-	-	0/13/13/13	0/0/0/0
3	DMA	B	501	2	-	0/13/13/13	0/0/0/0
4	SO4	C	302	-	-	0/0/0/0	0/0/0/0
4	SO4	C	303	-	-	0/0/0/0	0/0/0/0
4	SO4	C	304	-	-	0/0/0/0	0/0/0/0
3	DMA	C	500	-	-	0/13/13/13	0/0/0/0
3	DMA	C	501	2	-	0/13/13/13	0/0/0/0
3	DMA	D	500	-	-	0/13/13/13	0/0/0/0
3	DMA	D	501	2	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	DMA	C1-C2-C3	-4.06	120.05	126.71
3	B	501	DMA	C1-C2-C3	-3.95	120.24	126.71
3	A	501	DMA	C1-C2-C3	-3.75	120.57	126.71
3	D	501	DMA	C1-C2-C3	-3.61	120.78	126.71
3	C	500	DMA	C1-C2-C3	-3.23	121.41	126.71
3	B	500	DMA	PA-O3A-PB	-2.84	123.16	132.67
3	A	500	DMA	PA-O3A-PB	-2.71	123.59	132.67
3	C	500	DMA	PA-O3A-PB	-2.68	123.68	132.67
3	A	500	DMA	C1-C2-C3	-2.64	122.38	126.71
3	B	500	DMA	C1-C2-C3	-2.61	122.43	126.71
3	B	501	DMA	PA-O3A-PB	-2.47	124.39	132.67
3	D	500	DMA	PA-O3A-PB	-2.41	124.58	132.67
3	A	500	DMA	O1-C1-C2	-2.30	99.29	109.68
3	C	501	DMA	PA-O3A-PB	-2.28	125.02	132.67
3	D	500	DMA	C1-C2-C3	-2.24	123.04	126.71
3	A	501	DMA	PA-O3A-PB	-2.23	125.18	132.67
3	C	501	DMA	O3A-PA-O1	-2.19	97.14	102.94
3	D	501	DMA	C5-C3-C4	2.16	119.94	114.64
3	D	500	DMA	O3B-PB-O2B	2.16	115.61	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	DMA	1	0
3	C	500	DMA	1	0
3	C	501	DMA	2	0
3	D	501	DMA	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	303/310 (97%)	-0.15	6 (1%) 68 68	30, 47, 81, 119	0
1	B	303/310 (97%)	-0.11	12 (3%) 42 43	31, 56, 99, 130	0
1	C	301/310 (97%)	-0.06	8 (2%) 58 57	36, 56, 91, 130	0
1	D	299/310 (96%)	0.66	37 (12%) 5 5	43, 78, 133, 152	0
All	All	1206/1240 (97%)	0.09	63 (5%) 31 31	30, 58, 108, 152	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	SER	7.9
1	D	246	LEU	7.5
1	D	247	ASP	6.5
1	D	231	ILE	6.5
1	A	247	ASP	6.4
1	C	246	LEU	6.2
1	B	301	GLY	5.9
1	D	235	GLN	5.7
1	D	234	THR	5.6
1	C	247	ASP	5.4
1	B	247	ASP	5.3
1	D	298	LEU	5.2
1	D	245	HIS	4.9
1	C	249	ALA	4.8
1	D	300	LYS	4.5
1	B	246	LEU	4.5
1	D	65	LYS	4.3
1	D	69	ASN	4.2
1	A	248	SER	4.2
1	D	63	GLY	4.2
1	D	237	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	30	PHE	4.1
1	A	246	LEU	3.9
1	A	301	GLY	3.8
1	D	248	SER	3.8
1	D	238	GLU	3.5
1	D	204	ILE	3.5
1	D	105	ASN	3.4
1	D	244	THR	3.3
1	D	239	GLU	3.3
1	D	205	LYS	3.3
1	D	64	GLN	3.3
1	D	275	ASN	3.2
1	D	280	LEU	3.2
1	D	4	PRO	3.2
1	D	10	TYR	3.0
1	D	299	PHE	2.9
1	B	248	SER	2.8
1	D	236	ASP	2.8
1	C	171	ASN	2.8
1	B	233	VAL	2.7
1	B	300	LYS	2.7
1	B	238	GLU	2.6
1	D	68	SER	2.6
1	C	264	ASN	2.6
1	C	259	LEU	2.6
1	A	236	ASP	2.4
1	D	260	GLU	2.4
1	D	7	SER	2.4
1	B	-1	HIS	2.4
1	D	271	THR	2.3
1	B	245[A]	HIS	2.2
1	D	8	PHE	2.2
1	D	278	ASP	2.1
1	B	234	THR	2.1
1	D	282	PRO	2.1
1	D	11	ASN	2.1
1	B	28	GLU	2.0
1	D	286	LEU	2.0
1	C	244	THR	2.0
1	D	240	SER	2.0
1	A	238	GLU	2.0
1	D	232	ASP	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
3	DMA	D	500	14/14	0.84	0.22	0.69	107,117,120,123	0
4	SO4	C	302	5/5	0.97	0.14	0.40	79,81,92,94	0
3	DMA	C	500	14/14	0.99	0.12	-0.33	41,47,67,67	0
3	DMA	C	501	14/14	0.98	0.12	-0.47	44,56,61,71	0
3	DMA	A	500	14/14	0.99	0.12	-0.53	37,50,56,60	0
3	DMA	D	501	14/14	0.96	0.15	-0.54	51,79,86,90	0
3	DMA	A	501	14/14	0.99	0.13	-0.58	41,52,62,65	0
3	DMA	B	501	14/14	0.98	0.10	-0.63	44,61,69,69	0
3	DMA	B	500	14/14	0.98	0.10	-0.85	40,61,66,74	0
2	MG	C	401	1/1	0.92	0.05	-1.98	72,72,72,72	0
2	MG	D	400	1/1	0.91	0.17	-	62,62,62,62	0
2	MG	C	400	1/1	0.97	0.06	-	58,58,58,58	0
4	SO4	C	304	5/5	0.89	0.20	-	126,133,134,136	0
4	SO4	A	304	5/5	0.92	0.20	-	118,121,122,123	0
4	SO4	C	303	5/5	0.89	0.25	-	133,134,135,136	0
4	SO4	A	302	5/5	0.78	0.16	-	91,108,113,114	0
4	SO4	A	303	5/5	0.89	0.20	-	135,135,136,137	0
2	MG	B	400	1/1	0.95	0.08	-	59,59,59,59	0
4	SO4	B	302	5/5	0.91	0.34	-	153,154,155,155	0
2	MG	A	400	1/1	0.93	0.15	-	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.