



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:13 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

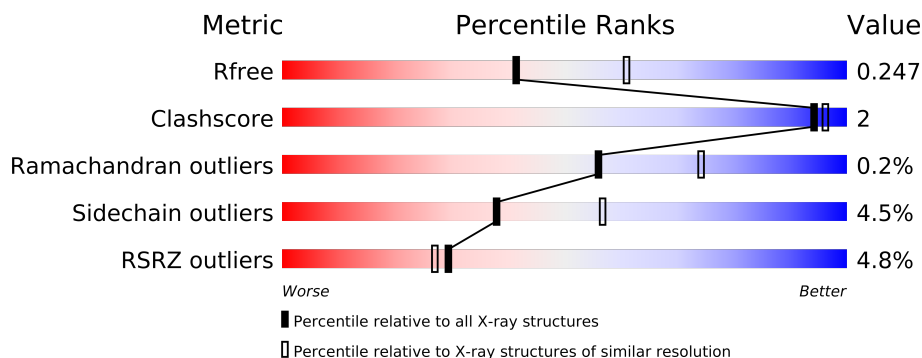
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	310	
1	B	310	
1	C	310	
1	D	310	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	303	-	X
4	SO4	A	304	-	X
4	SO4	C	303	-	X
4	SO4	C	304	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10049 atoms, of which 0 are hydrogen and 0 are deuterium.

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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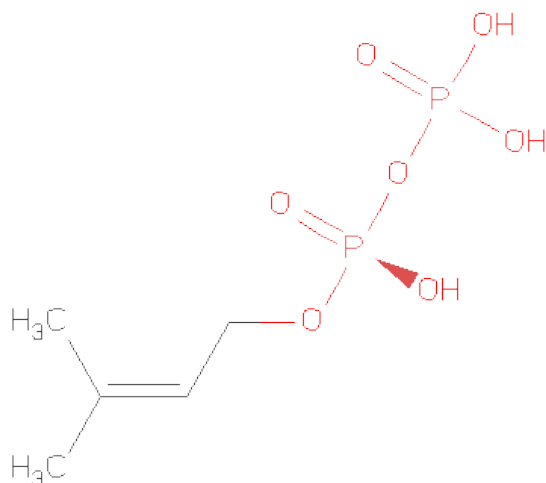
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	EXPRESSION TAG	UNP O25583
C	-6	HIS	-	EXPRESSION TAG	UNP O25583
C	-5	HIS	-	EXPRESSION TAG	UNP O25583
C	-4	HIS	-	EXPRESSION TAG	UNP O25583
C	-3	HIS	-	EXPRESSION TAG	UNP O25583
C	-2	HIS	-	EXPRESSION 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: C₅H₁₂O₇P₂).



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: O₄S).



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		

3 Residue-property plots

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.

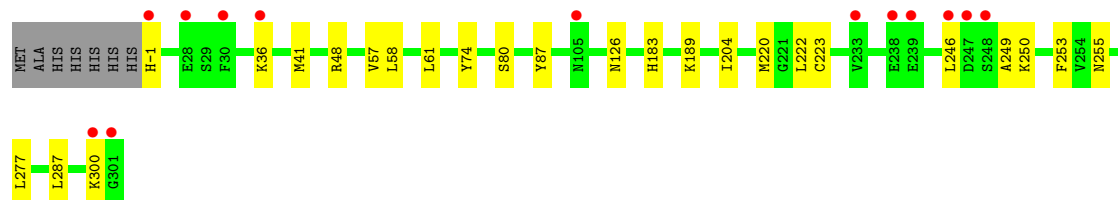
- Molecule 1: Geranyltranstransferase(IspA)

Chain A: 



- Molecule 1: Geranyltranstransferase(IspA)

Chain B: 



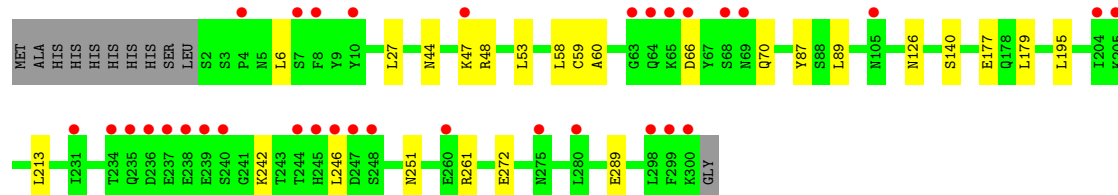
- Molecule 1: Geranyltranstransferase(IspA)

Chain C: 



- Molecule 1: Geranyltranstransferase(IspA)

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.243 0.220 , 0.247	Depositor DCC
R_{free} test set	3076 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	18	1	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:250[A]:LYS:HG2	1:A:251[A]:ASN:N	2.32	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	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%)	30	43
All	All	1207/1240 (97%)	1165 (96%)	40 (3%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

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

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	271/272 (100%)	260 (96%)	11 (4%)	41	61
1	B	268/272 (98%)	255 (95%)	13 (5%)	35	53
1	C	267/272 (98%)	252 (94%)	15 (6%)	30	45
1	D	263/272 (97%)	253 (96%)	10 (4%)	44	65
All	All	1069/1088 (98%)	1020 (95%)	49 (5%)	38	55

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
1	C	97	MET
1	C	126	ASN
1	C	140	SER

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Mol	Chain	Res	Type
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 chains 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 ⓘ

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	0.17	0	6,6,6	0.16	0
4	SO4	A	303	-	4,4,4	0.20	0	6,6,6	0.11	0
4	SO4	A	304	-	4,4,4	0.21	0	6,6,6	0.13	0
3	DMA	A	500	-	13,13,13	0.64	0	19,19,19	1.63	4 (21%)
3	DMA	A	501	2	13,13,13	0.64	0	19,19,19	1.61	3 (15%)
4	SO4	B	302	-	4,4,4	0.19	0	6,6,6	0.09	0
3	DMA	B	500	-	13,13,13	0.62	0	19,19,19	1.43	2 (10%)
3	DMA	B	501	2	13,13,13	0.59	0	19,19,19	1.52	3 (15%)
4	SO4	C	302	-	4,4,4	0.29	0	6,6,6	0.17	0
4	SO4	C	303	-	4,4,4	0.20	0	6,6,6	0.07	0
4	SO4	C	304	-	4,4,4	0.18	0	6,6,6	0.06	0
3	DMA	C	500	-	13,13,13	0.71	0	19,19,19	1.56	3 (15%)
3	DMA	C	501	2	13,13,13	0.57	0	19,19,19	1.68	3 (15%)
3	DMA	D	500	-	13,13,13	0.74	0	19,19,19	1.22	3 (15%)
3	DMA	D	501	2	13,13,13	0.67	0	19,19,19	1.42	2 (10%)

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 (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	DMA	C1-C2-C3	-4.36	120.05	126.84
3	B	501	DMA	C1-C2-C3	-4.24	120.24	126.84
3	A	501	DMA	C1-C2-C3	-4.03	120.57	126.84
3	D	501	DMA	C1-C2-C3	-3.89	120.78	126.84
3	A	500	DMA	PA-O1-C1	3.54	126.02	120.36
3	C	500	DMA	C1-C2-C3	-3.49	121.41	126.84
3	A	501	DMA	PA-O1-C1	-3.37	114.96	120.36
3	C	501	DMA	PA-O1-C1	-3.05	115.48	120.36
3	B	500	DMA	PA-O3A-PB	-2.91	123.16	131.68
3	C	500	DMA	PA-O1-C1	2.88	124.96	120.36
3	A	500	DMA	C1-C2-C3	-2.87	122.38	126.84
3	B	500	DMA	C1-C2-C3	-2.83	122.43	126.84
3	A	500	DMA	PA-O3A-PB	-2.76	123.59	131.68
3	C	500	DMA	PA-O3A-PB	-2.73	123.68	131.68
3	B	501	DMA	PA-O3A-PB	-2.49	124.39	131.68
3	D	500	DMA	C1-C2-C3	-2.44	123.04	126.84
3	D	500	DMA	PA-O3A-PB	-2.42	124.58	131.68
3	A	500	DMA	O1-C1-C2	-2.35	99.29	109.94
3	C	501	DMA	PA-O3A-PB	-2.27	125.02	131.68
3	A	501	DMA	PA-O3A-PB	-2.22	125.18	131.68
3	D	501	DMA	C5-C3-C4	2.09	119.94	114.62
3	B	501	DMA	PA-O1-C1	-2.06	117.07	120.36
3	D	500	DMA	O3B-PB-O2B	2.05	115.61	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/310 (97%)	-0.13	4 (1%) 74 73	30, 47, 81, 119	0
1	B	303/310 (97%)	-0.10	13 (4%) 34 32	31, 56, 99, 130	0
1	C	301/310 (97%)	-0.03	8 (2%) 52 49	36, 56, 91, 130	0
1	D	299/310 (96%)	0.63	33 (11%) 6 5	43, 78, 133, 152	0
All	All	1206/1240 (97%)	0.09	58 (4%) 29 27	30, 58, 108, 152	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	SER	7.5
1	A	247	ASP	7.0
1	D	246	LEU	6.9
1	C	246	LEU	6.6
1	D	231	ILE	6.0
1	C	247	ASP	5.4
1	B	247	ASP	5.2
1	D	247	ASP	5.1
1	D	235	GLN	5.1
1	D	234	THR	5.0
1	D	300	LYS	4.9
1	D	237	GLU	4.7
1	D	245	HIS	4.7
1	B	301	GLY	4.6
1	C	249	ALA	4.6
1	D	298	LEU	4.6
1	A	246	LEU	4.4
1	B	30	PHE	4.2
1	D	65	LYS	4.1
1	D	248	SER	3.9
1	B	246	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	63	GLY	3.8
1	D	69	ASN	3.8
1	A	248	SER	3.7
1	D	299	PHE	3.6
1	D	64	GLN	3.5
1	D	10	TYR	3.4
1	D	244	THR	3.3
1	D	105	ASN	3.3
1	C	259	LEU	3.2
1	D	205	LYS	3.2
1	D	204	ILE	3.1
1	A	301	GLY	3.0
1	D	236	ASP	2.9
1	D	238	GLU	2.9
1	D	239	GLU	2.8
1	D	4	PRO	2.8
1	B	300	LYS	2.8
1	D	280	LEU	2.7
1	D	275	ASN	2.7
1	D	68	SER	2.6
1	B	248	SER	2.5
1	B	238	GLU	2.5
1	C	250	LYS	2.4
1	D	7	SER	2.4
1	D	240	SER	2.4
1	B	-1	HIS	2.2
1	C	264	ASN	2.2
1	B	239	GLU	2.1
1	C	171	ASN	2.1
1	D	260	GLU	2.1
1	B	233	VAL	2.1
1	B	105	ASN	2.1
1	D	47	LYS	2.1
1	B	28	GLU	2.1
1	B	36	LYS	2.0
1	D	8	PHE	2.0
1	D	66	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	A	304	5/5	0.21	10.02	118,121,122,123	0
4	SO4	A	303	5/5	0.22	8.09	135,135,136,137	0
4	SO4	C	304	5/5	0.19	3.68	126,133,134,136	0
4	SO4	C	303	5/5	0.26	3.17	133,134,135,136	0
4	SO4	A	302	5/5	0.14	0.73	91,108,113,114	0
3	DMA	D	500	14/14	0.21	0.50	107,117,120,123	0
4	SO4	B	302	5/5	0.28	0.39	153,154,155,155	0
4	SO4	C	302	5/5	0.13	0.10	79,81,92,94	0
2	MG	D	400	1/1	0.17	-0.26	62,62,62,62	0
3	DMA	A	500	14/14	0.12	-0.33	37,50,56,60	0
3	DMA	C	501	14/14	0.12	-0.34	44,56,61,71	0
3	DMA	C	500	14/14	0.12	-0.36	41,47,67,67	0
3	DMA	D	501	14/14	0.15	-0.45	51,79,86,90	0
2	MG	A	400	1/1	0.14	-0.48	49,49,49,49	0
3	DMA	B	501	14/14	0.11	-0.61	44,61,69,69	0
3	DMA	A	501	14/14	0.12	-0.66	41,52,62,65	0
3	DMA	B	500	14/14	0.10	-0.79	40,61,66,74	0
2	MG	C	400	1/1	0.07	-1.00	58,58,58,58	0
2	MG	B	400	1/1	0.08	-1.09	59,59,59,59	0
2	MG	C	401	1/1	0.05	-1.86	72,72,72,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.