



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 03:49 PM JST

PDB ID : 5XK7
Title : Crystal structure of Isosesquilavandulyl Diphosphate Synthase from Streptomyces sp. strain CNH-189 in complex with DMAPP
Authors : Ko, T.P.; Guo, R.T.; Liu, W.; Chen, C.C.; Gao, J.
Deposited on : 2017-05-05
Resolution : 1.91 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

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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

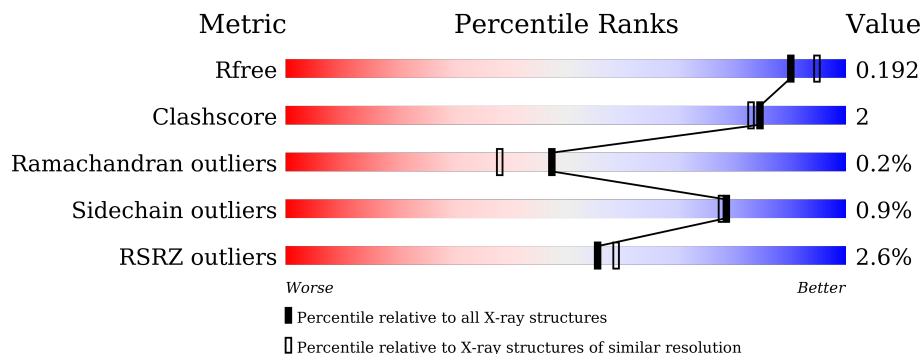
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 ≥ 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	232	 4% 88% 6% 6%
1	B	232	 % 82% 9% 9%
1	C	232	 4% 89% 5% 6%
1	D	232	 % 84% 6% 10%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7960 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 Undecaprenyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1753	1116	291	330	16	0	2	0
1	B	210	1701	1082	281	321	17	0	4	0
1	C	217	1761	1123	291	332	15	0	4	0
1	D	209	1688	1074	277	321	16	0	4	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	expression tag	UNP M4T4U9
A	-13	ALA	-	expression tag	UNP M4T4U9
A	-12	HIS	-	expression tag	UNP M4T4U9
A	-11	HIS	-	expression tag	UNP M4T4U9
A	-10	HIS	-	expression tag	UNP M4T4U9
A	-9	HIS	-	expression tag	UNP M4T4U9
A	-8	HIS	-	expression tag	UNP M4T4U9
A	-7	HIS	-	expression tag	UNP M4T4U9
A	-6	VAL	-	expression tag	UNP M4T4U9
A	-5	ASP	-	expression tag	UNP M4T4U9
A	-4	ASP	-	expression tag	UNP M4T4U9
A	-3	ASP	-	expression tag	UNP M4T4U9
A	-2	ASP	-	expression tag	UNP M4T4U9
A	-1	LYS	-	expression tag	UNP M4T4U9
A	0	MET	-	expression tag	UNP M4T4U9
B	-14	MET	-	expression tag	UNP M4T4U9
B	-13	ALA	-	expression tag	UNP M4T4U9
B	-12	HIS	-	expression tag	UNP M4T4U9
B	-11	HIS	-	expression tag	UNP M4T4U9
B	-10	HIS	-	expression tag	UNP M4T4U9
B	-9	HIS	-	expression tag	UNP M4T4U9

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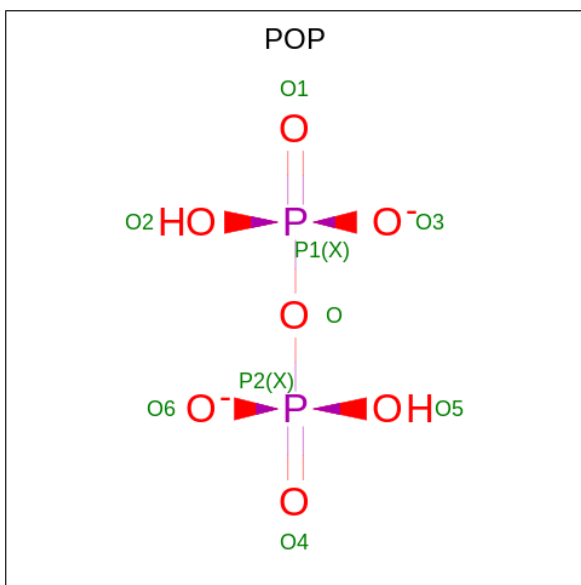
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP M4T4U9
B	-7	HIS	-	expression tag	UNP M4T4U9
B	-6	VAL	-	expression tag	UNP M4T4U9
B	-5	ASP	-	expression tag	UNP M4T4U9
B	-4	ASP	-	expression tag	UNP M4T4U9
B	-3	ASP	-	expression tag	UNP M4T4U9
B	-2	ASP	-	expression tag	UNP M4T4U9
B	-1	LYS	-	expression tag	UNP M4T4U9
B	0	MET	-	expression tag	UNP M4T4U9
C	-14	MET	-	expression tag	UNP M4T4U9
C	-13	ALA	-	expression tag	UNP M4T4U9
C	-12	HIS	-	expression tag	UNP M4T4U9
C	-11	HIS	-	expression tag	UNP M4T4U9
C	-10	HIS	-	expression tag	UNP M4T4U9
C	-9	HIS	-	expression tag	UNP M4T4U9
C	-8	HIS	-	expression tag	UNP M4T4U9
C	-7	HIS	-	expression tag	UNP M4T4U9
C	-6	VAL	-	expression tag	UNP M4T4U9
C	-5	ASP	-	expression tag	UNP M4T4U9
C	-4	ASP	-	expression tag	UNP M4T4U9
C	-3	ASP	-	expression tag	UNP M4T4U9
C	-2	ASP	-	expression tag	UNP M4T4U9
C	-1	LYS	-	expression tag	UNP M4T4U9
C	0	MET	-	expression tag	UNP M4T4U9
D	-14	MET	-	expression tag	UNP M4T4U9
D	-13	ALA	-	expression tag	UNP M4T4U9
D	-12	HIS	-	expression tag	UNP M4T4U9
D	-11	HIS	-	expression tag	UNP M4T4U9
D	-10	HIS	-	expression tag	UNP M4T4U9
D	-9	HIS	-	expression tag	UNP M4T4U9
D	-8	HIS	-	expression tag	UNP M4T4U9
D	-7	HIS	-	expression tag	UNP M4T4U9
D	-6	VAL	-	expression tag	UNP M4T4U9
D	-5	ASP	-	expression tag	UNP M4T4U9
D	-4	ASP	-	expression tag	UNP M4T4U9
D	-3	ASP	-	expression tag	UNP M4T4U9
D	-2	ASP	-	expression tag	UNP M4T4U9
D	-1	LYS	-	expression tag	UNP M4T4U9
D	0	MET	-	expression tag	UNP M4T4U9

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

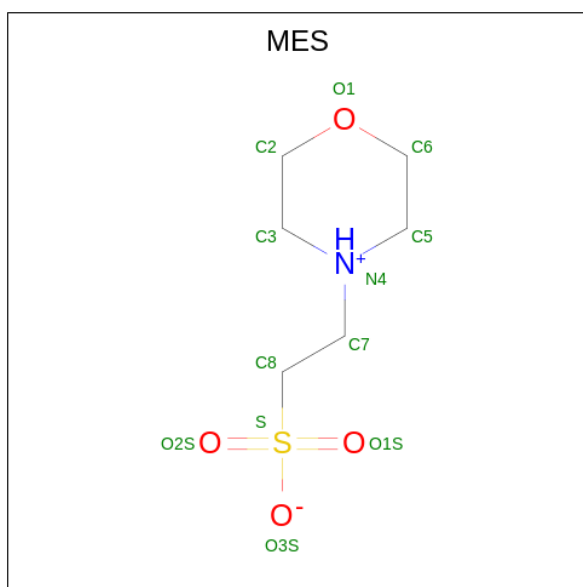
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



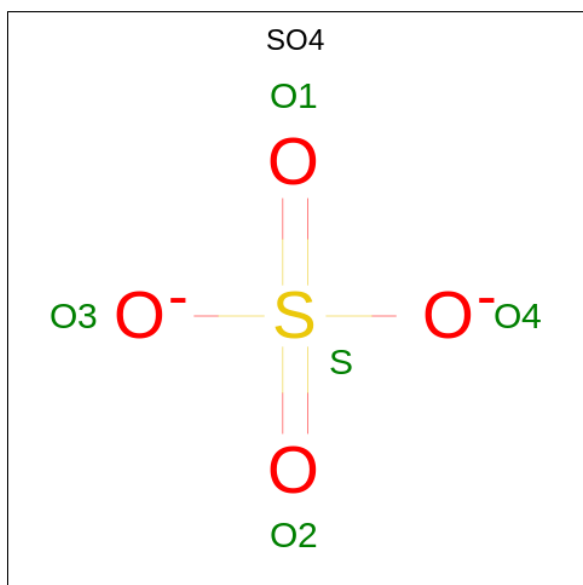
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	A	1	Total O P 13 10 3	0	1
3	B	1	Total O P 9 7 2	0	0
3	C	1	Total O P 9 7 2	0	0
3	D	1	Total O P 9 7 2	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



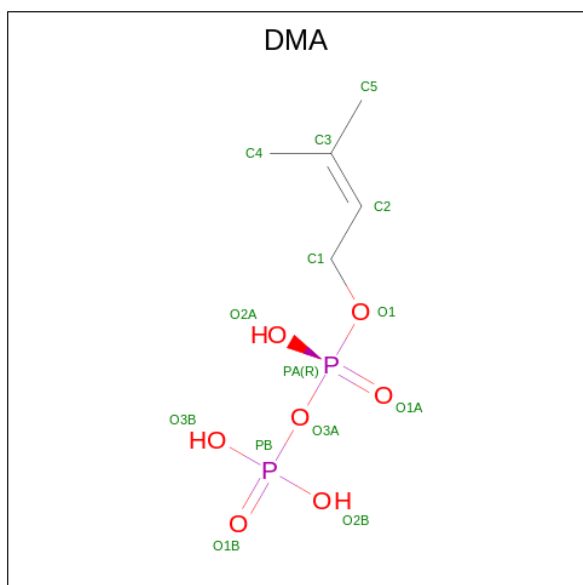
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is DIMETHYLALLYL DIPHOSPHATE (three-letter code: DMA) (formula: $C_5H_{12}O_7P_2$).



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

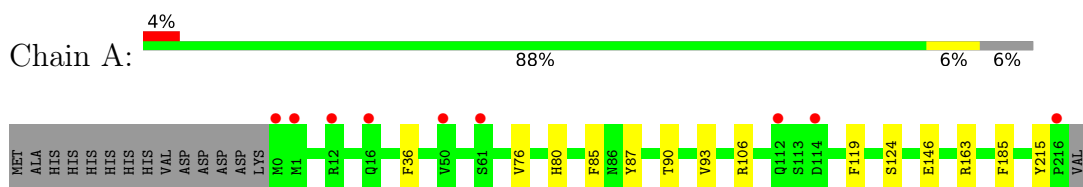
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	212	Total O 212 212	0	0
7	B	205	Total O 205 205	0	0
7	C	250	Total O 250 250	0	0
7	D	237	Total O 237 237	0	0

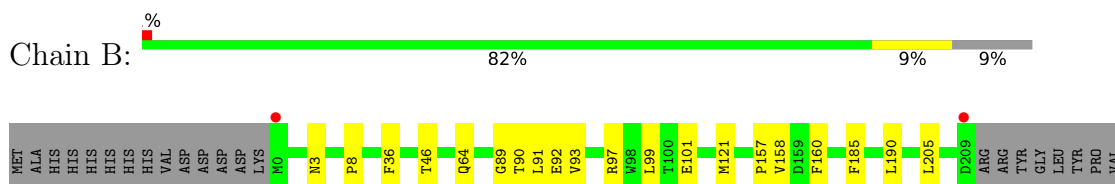
3 Residue-property plots [i](#)

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.

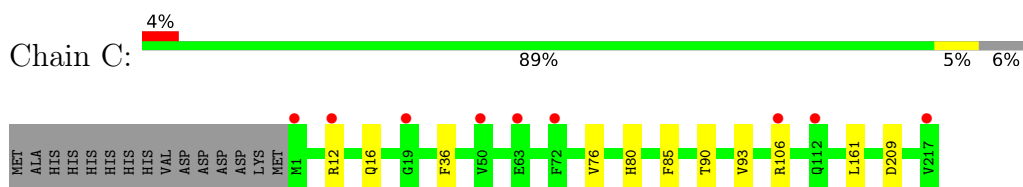
- Molecule 1: Undecaprenyl diphosphate synthase



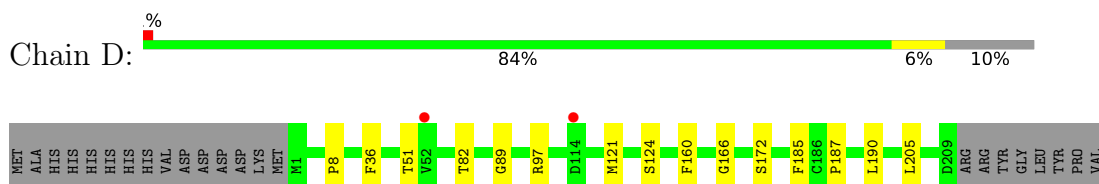
- Molecule 1: Undecaprenyl diphosphate synthase



- Molecule 1: Undecaprenyl diphosphate synthase



- Molecule 1: Undecaprenyl diphosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.92Å 120.65Å 126.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.73 – 1.91 24.73 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.73-1.91) 94.8 (24.73-1.91)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.90Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.169 , 0.192 0.169 , 0.192	Depositor DCC
R_{free} test set	1999 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtrriage
Anisotropy	0.684	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.034 for -h,l,k	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7960	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

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

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	0.30	0/1801	0.49	0/2440
1	B	0.35	1/1752 (0.1%)	0.50	0/2372
1	C	0.30	0/1815	0.50	0/2460
1	D	0.31	0/1739	0.50	0/2356
All	All	0.32	1/7107 (0.0%)	0.50	0/9628

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	GLU	CD-OE2	7.06	1.33	1.25

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	1753	0	1703	8	0
1	B	1701	0	1660	12	0
1	C	1761	0	1719	6	0
1	D	1688	0	1643	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	22	0	0	0	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
4	A	12	0	12	1	0
4	B	12	0	12	1	0
4	C	12	0	12	0	0
4	D	12	0	12	1	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
6	B	14	0	9	0	0
6	C	14	0	9	0	0
6	D	14	0	9	1	0
7	A	212	0	0	1	0
7	B	205	0	0	3	0
7	C	250	0	0	2	0
7	D	237	0	0	1	0
All	All	7960	0	6800	32	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 (32) 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:209:ASP:OD2	7:C:401:HOH:O	2.02	0.78
1:C:209:ASP:OD1	7:C:402:HOH:O	2.05	0.73
1:D:8:PRO:HB3	1:D:190:LEU:HD22	1.81	0.63
1:D:82:THR:OG1	7:D:401:HOH:O	2.15	0.63
1:A:85:PHE:O	1:A:106:ARG:HG3	2.05	0.56
1:B:8:PRO:HB3	1:B:190:LEU:HD22	1.88	0.55
1:C:85:PHE:O	1:C:106:ARG:HG3	2.07	0.54
1:D:160:PHE:HB3	1:D:205:LEU:HD13	1.90	0.53
1:B:157:PRO:HG2	7:B:550:HOH:O	2.09	0.52
1:B:46:THR:OG1	7:B:401:HOH:O	2.19	0.52
1:D:185:PHE:O	4:D:304:MES:H82	2.10	0.52
1:A:185:PHE:O	4:A:304:MES:H81	2.10	0.51
1:A:146:GLU:OE2	7:A:401:HOH:O	2.19	0.51
1:A:76:VAL:O	1:A:80:HIS:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASN:OD1	1:B:158:VAL:HA	2.12	0.48
1:C:76:VAL:O	1:C:80:HIS:HB3	2.13	0.48
1:B:185:PHE:O	4:B:304:MES:H82	2.14	0.47
1:A:215:TYR:HD2	1:B:64:GLN:NE2	2.15	0.45
1:B:160:PHE:HB3	1:B:205:LEU:HD13	1.99	0.45
1:B:91:LEU:O	1:B:99:LEU:HD11	2.17	0.45
1:B:3:ASN:HB3	7:B:401:HOH:O	2.17	0.44
1:B:89:GLY:HA3	1:B:121:MET:O	2.16	0.43
1:B:97[B]:ARG:NH2	1:B:101:GLU:OE2	2.42	0.43
1:A:90:THR:O	1:A:93:VAL:HG22	2.19	0.42
1:C:90:THR:O	1:C:93:VAL:HG22	2.20	0.42
1:C:12:ARG:HH21	1:C:16:GLN:HE22	1.68	0.40
1:B:90:THR:O	1:B:93:VAL:HG22	2.20	0.40
1:A:87:TYR:HA	1:A:119:PHE:O	2.21	0.40
1:D:51:THR:O	6:D:303:DMA:H51	2.21	0.40
1:D:89:GLY:HA3	1:D:121:MET:O	2.20	0.40
1:D:166:GLY:HA2	1:D:187:PRO:HA	2.03	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	217/232 (94%)	214 (99%)	2 (1%)	1 (0%)	29	18
1	B	212/232 (91%)	208 (98%)	4 (2%)	0	100	100
1	C	219/232 (94%)	216 (99%)	3 (1%)	0	100	100
1	D	211/232 (91%)	206 (98%)	4 (2%)	1 (0%)	29	18
All	All	859/928 (93%)	844 (98%)	13 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	SER
1	A	124	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/204 (94%)	191 (100%)	1 (0%)	88	89
1	B	188/204 (92%)	187 (100%)	1 (0%)	88	89
1	C	194/204 (95%)	192 (99%)	2 (1%)	76	75
1	D	187/204 (92%)	183 (98%)	4 (2%)	53	46
All	All	761/816 (93%)	753 (99%)	8 (1%)	78	72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	B	36	PHE
1	C	36	PHE
1	C	161	LEU
1	D	36	PHE
1	D	97	ARG
1	D	172[A]	SER
1	D	172[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	B	84	ASN
1	C	16	GLN

5.3.3 RNA [i](#)

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 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	MES	A	304	-	12,12,12	2.17	1 (8%)	14,16,16	2.52	5 (35%)
3	POP	A	303[A]	-	6,8,8	0.77	0	13,13,13	1.50	2 (15%)
6	DMA	C	303	2	11,13,13	1.11	1 (9%)	15,19,19	1.50	3 (20%)
3	POP	C	302	2	6,8,8	0.74	0	13,13,13	1.17	1 (7%)
5	SO4	A	305	-	4,4,4	0.14	0	6,6,6	0.06	0
4	MES	D	304	-	12,12,12	2.22	1 (8%)	14,16,16	2.09	5 (35%)
5	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.05	0
6	DMA	D	303	2	11,13,13	1.18	1 (9%)	15,19,19	1.39	2 (13%)
6	DMA	B	303	2	11,13,13	1.15	1 (9%)	15,19,19	1.21	2 (13%)
4	MES	C	304	-	12,12,12	2.12	1 (8%)	14,16,16	1.89	5 (35%)
3	POP	B	302	2	6,8,8	0.71	0	13,13,13	1.12	1 (7%)
3	POP	A	303[B]	-	6,8,8	0.78	0	13,13,13	1.12	2 (15%)
4	MES	B	304	-	12,12,12	2.32	1 (8%)	14,16,16	2.37	6 (42%)
3	POP	D	302	2	6,8,8	0.66	0	13,13,13	1.04	2 (15%)
3	POP	A	302	2	6,8,8	0.72	0	13,13,13	1.20	1 (7%)

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	MES	A	304	-	-	5/6/14/14	0/1/1/1
3	POP	A	303[A]	-	-	0/6/6/6	-
6	DMA	C	303	2	-	5/13/13/13	-
3	POP	C	302	2	-	2/6/6/6	-
4	MES	D	304	-	-	5/6/14/14	0/1/1/1
6	DMA	D	303	2	-	4/13/13/13	-
6	DMA	B	303	2	-	3/13/13/13	-
4	MES	C	304	-	-	4/6/14/14	0/1/1/1
3	POP	B	302	2	-	1/6/6/6	-
3	POP	A	303[B]	-	-	1/6/6/6	-
4	MES	B	304	-	-	5/6/14/14	0/1/1/1
3	POP	D	302	2	-	1/6/6/6	-
3	POP	A	302	2	-	3/6/6/6	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	MES	C8-S	-7.75	1.66	1.77
4	D	304	MES	C8-S	-7.45	1.66	1.77
4	A	304	MES	C8-S	-7.25	1.67	1.77
4	C	304	MES	C8-S	-7.05	1.67	1.77
6	D	303	DMA	O1-C1	-2.50	1.40	1.43
6	B	303	DMA	O1-C1	-2.39	1.40	1.43
6	C	303	DMA	O1-C1	-2.05	1.40	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	304	MES	C5-N4-C3	5.14	120.40	108.83
4	A	304	MES	C5-N4-C3	5.04	120.18	108.83
3	A	303[A]	POP	P2-O-P1	-4.20	118.41	132.83
4	A	304	MES	C6-C5-N4	-3.98	104.06	110.10
4	D	304	MES	C5-N4-C3	3.98	117.79	108.83
4	A	304	MES	C7-N4-C5	3.97	121.40	111.23
4	B	304	MES	C6-C5-N4	-3.96	104.10	110.10
6	D	303	DMA	C1-C2-C3	-3.65	120.84	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	303	DMA	C1-C2-C3	-3.62	120.89	126.75
6	B	303	DMA	C1-C2-C3	-3.33	121.36	126.75
4	D	304	MES	C7-N4-C3	3.02	118.96	111.23
6	C	303	DMA	PA-O3A-PB	-3.02	122.48	132.83
3	A	302	POP	P2-O-P1	-2.95	122.70	132.83
4	C	304	MES	C5-N4-C3	2.93	115.43	108.83
4	C	304	MES	C7-N4-C3	2.91	118.69	111.23
4	A	304	MES	O1S-S-C8	2.86	110.36	106.92
4	B	304	MES	C7-N4-C3	2.85	118.52	111.23
4	D	304	MES	O3S-S-C8	2.83	110.35	105.77
4	A	304	MES	C7-N4-C3	2.81	118.42	111.23
4	D	304	MES	C6-C5-N4	-2.74	105.95	110.10
4	B	304	MES	C7-N4-C5	2.72	118.20	111.23
4	C	304	MES	C6-C5-N4	-2.60	106.17	110.10
4	D	304	MES	C7-N4-C5	2.54	117.73	111.23
3	D	302	POP	P2-O-P1	-2.54	124.12	132.83
3	B	302	POP	P2-O-P1	-2.51	124.22	132.83
4	B	304	MES	O2S-S-C8	2.50	109.93	106.92
4	C	304	MES	O2S-S-C8	2.44	109.85	106.92
6	D	303	DMA	C5-C3-C4	2.40	119.90	114.60
3	A	303[A]	POP	O2-P1-O	2.38	112.62	104.64
3	A	303[B]	POP	O2-P1-O	2.38	112.62	104.64
3	A	303[B]	POP	P2-O-P1	-2.37	124.69	132.83
6	B	303	DMA	C5-C3-C4	2.33	119.74	114.60
4	B	304	MES	O3S-S-C8	2.28	109.46	105.77
3	D	302	POP	O2-P1-O	2.19	111.97	104.64
6	C	303	DMA	C5-C3-C4	2.11	119.26	114.60
3	C	302	POP	P2-O-P1	-2.10	125.60	132.83
4	C	304	MES	C2-C3-N4	-2.04	107.01	110.10

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	POP	P1-O-P2-O6
3	A	303[B]	POP	P1-O-P2-O5
3	B	302	POP	P1-O-P2-O6
3	C	302	POP	P1-O-P2-O6
3	D	302	POP	P1-O-P2-O6
4	A	304	MES	C8-C7-N4-C5
4	B	304	MES	N4-C7-C8-S
4	B	304	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
4	B	304	MES	C7-C8-S-O3S
4	C	304	MES	C8-C7-N4-C3
4	D	304	MES	C8-C7-N4-C3
4	D	304	MES	C7-C8-S-O2S
4	D	304	MES	C7-C8-S-O3S
6	D	303	DMA	C1-O1-PA-O3A
4	A	304	MES	C7-C8-S-O3S
4	B	304	MES	C8-C7-N4-C5
4	C	304	MES	C8-C7-N4-C5
4	D	304	MES	C8-C7-N4-C5
6	C	303	DMA	PA-O3A-PB-O1B
6	B	303	DMA	C1-O1-PA-O3A
6	B	303	DMA	PB-O3A-PA-O1A
6	B	303	DMA	C1-O1-PA-O2A
6	C	303	DMA	C1-O1-PA-O1A
6	D	303	DMA	C1-O1-PA-O1A
4	A	304	MES	C7-C8-S-O1S
4	A	304	MES	C7-C8-S-O2S
4	B	304	MES	C7-C8-S-O2S
4	C	304	MES	C7-C8-S-O1S
4	D	304	MES	C7-C8-S-O1S
6	D	303	DMA	PB-O3A-PA-O2A
4	A	304	MES	C8-C7-N4-C3
3	A	302	POP	P1-O-P2-O5
3	C	302	POP	P1-O-P2-O5
6	C	303	DMA	PA-O3A-PB-O2B
6	C	303	DMA	PA-O3A-PB-O3B
6	C	303	DMA	C1-O1-PA-O3A
6	D	303	DMA	PB-O3A-PA-O1A
4	C	304	MES	C7-C8-S-O3S
3	A	302	POP	P1-O-P2-O4

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	MES	1	0
4	D	304	MES	1	0
6	D	303	DMA	1	0
4	B	304	MES	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, 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	217/232 (93%)	-0.02	9 (4%) 37 40	24, 35, 58, 107	0
1	B	210/232 (90%)	-0.16	2 (0%) 82 84	24, 33, 50, 105	0
1	C	217/232 (93%)	-0.03	9 (4%) 37 40	22, 32, 56, 92	0
1	D	209/232 (90%)	-0.21	2 (0%) 82 84	22, 32, 48, 72	0
All	All	853/928 (91%)	-0.10	22 (2%) 56 59	22, 33, 55, 107	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	VAL	6.0
1	B	209	ASP	5.2
1	A	0	MET	5.2
1	C	112	GLN	4.0
1	B	0	MET	3.7
1	C	19	GLY	3.5
1	A	112	GLN	3.1
1	A	50	VAL	2.8
1	A	1	MET	2.6
1	A	12	ARG	2.6
1	A	16	GLN	2.6
1	A	114	ASP	2.6
1	A	216	PRO	2.5
1	D	52	VAL	2.5
1	C	12	ARG	2.4
1	C	1	MET	2.3
1	C	63	GLU	2.2
1	C	72	PHE	2.2
1	C	106	ARG	2.2
1	C	50	VAL	2.2
1	D	114	ASP	2.1
1	A	61	SER	2.1

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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	301	1/1	0.76	0.13	65,65,65,65	0
4	MES	B	304	12/12	0.84	0.28	74,79,80,80	0
5	SO4	C	305	5/5	0.84	0.21	104,104,105,106	0
5	SO4	A	305	5/5	0.85	0.48	115,116,116,117	0
2	MG	C	301	1/1	0.87	0.10	56,56,56,56	0
3	POP	A	302	9/9	0.89	0.16	77,80,82,83	0
3	POP	A	303[A]	9/9	0.91	0.19	48,49,51,55	4
3	POP	A	303[B]	9/9	0.91	0.19	43,48,51,55	4
4	MES	A	304	12/12	0.91	0.22	59,70,73,73	0
4	MES	D	304	12/12	0.92	0.21	62,73,78,78	0
4	MES	C	304	12/12	0.95	0.15	42,58,66,66	0
3	POP	C	302	9/9	0.95	0.12	55,56,59,62	0
6	DMA	C	303	14/14	0.95	0.12	50,56,63,63	0
6	DMA	B	303	14/14	0.98	0.11	30,35,39,40	0
2	MG	B	301	1/1	0.98	0.08	32,32,32,32	0
6	DMA	D	303	14/14	0.98	0.13	26,30,35,36	0
3	POP	B	302	9/9	0.99	0.06	27,33,34,35	0
2	MG	D	301	1/1	0.99	0.10	26,26,26,26	0
3	POP	D	302	9/9	0.99	0.09	26,27,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.