



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 06:01 AM EDT

PDB ID : 5IMP
Title : Crystal structure of N299A Aspergillus terreus aristolochene synthase complexed with (1S,8S,9aR)-1,9a-dimethyl-8-(prop-1-en-2-yl)decahydroquinolizin-5-ium
Authors : Chen, M.; Christianson, D.W.
Deposited on : 2016-03-06
Resolution : 2.04 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 : 2.35.1
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) : 2.35.1

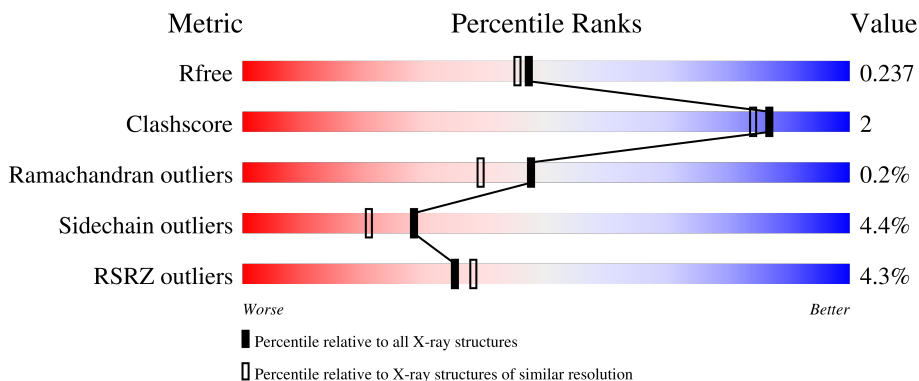
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	314	 91%
1	B	314	 % 91% 5%
1	C	314	 % 88% 8%
1	D	314	 14% 87% 9%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10968 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 Aristolochene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2467	1575	418	458	16	0	2	0
1	B	304	2456	1569	414	457	16	0	1	0
1	C	304	2464	1574	417	457	16	0	2	0
1	D	304	2456	1569	414	457	16	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

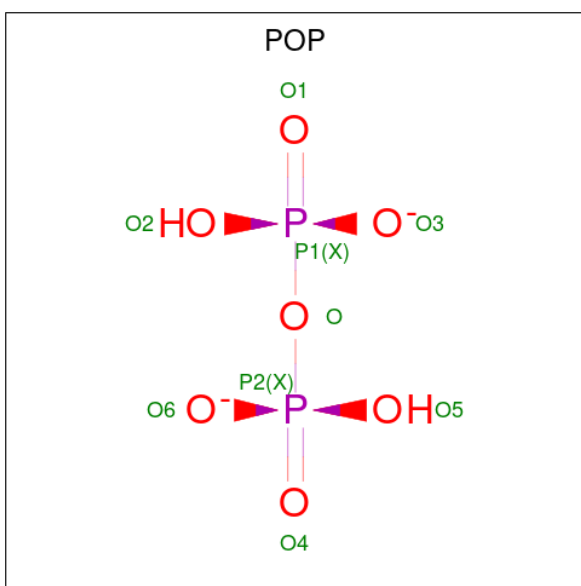
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9UR08
A	2	HIS	-	expression tag	UNP Q9UR08
A	3	HIS	-	expression tag	UNP Q9UR08
A	4	HIS	-	expression tag	UNP Q9UR08
A	5	HIS	-	expression tag	UNP Q9UR08
A	6	HIS	-	expression tag	UNP Q9UR08
A	7	HIS	-	expression tag	UNP Q9UR08
A	299	ALA	ASN	engineered mutation	UNP Q9UR08
B	1	MET	-	initiating methionine	UNP Q9UR08
B	2	HIS	-	expression tag	UNP Q9UR08
B	3	HIS	-	expression tag	UNP Q9UR08
B	4	HIS	-	expression tag	UNP Q9UR08
B	5	HIS	-	expression tag	UNP Q9UR08
B	6	HIS	-	expression tag	UNP Q9UR08
B	7	HIS	-	expression tag	UNP Q9UR08
B	299	ALA	ASN	engineered mutation	UNP Q9UR08
C	1	MET	-	initiating methionine	UNP Q9UR08
C	2	HIS	-	expression tag	UNP Q9UR08
C	3	HIS	-	expression tag	UNP Q9UR08
C	4	HIS	-	expression tag	UNP Q9UR08
C	5	HIS	-	expression tag	UNP Q9UR08

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	HIS	-	expression tag	UNP Q9UR08
C	7	HIS	-	expression tag	UNP Q9UR08
C	299	ALA	ASN	engineered mutation	UNP Q9UR08
D	1	MET	-	initiating methionine	UNP Q9UR08
D	2	HIS	-	expression tag	UNP Q9UR08
D	3	HIS	-	expression tag	UNP Q9UR08
D	4	HIS	-	expression tag	UNP Q9UR08
D	5	HIS	-	expression tag	UNP Q9UR08
D	6	HIS	-	expression tag	UNP Q9UR08
D	7	HIS	-	expression tag	UNP Q9UR08
D	299	ALA	ASN	engineered mutation	UNP Q9UR08

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).

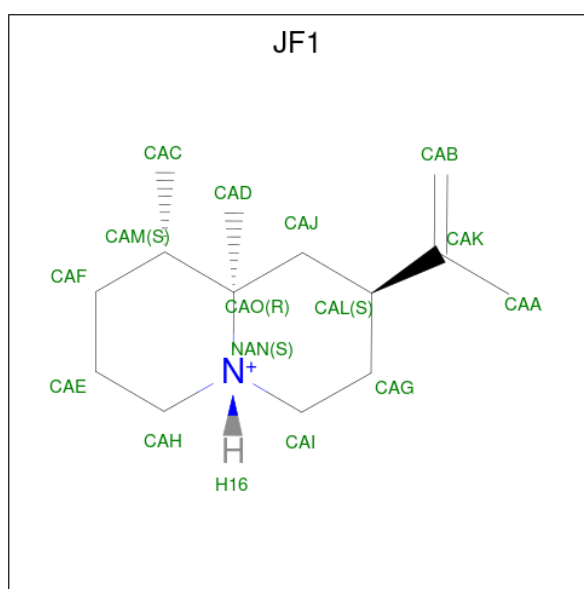


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 9 7 2	0	0
2	B	1	Total O P 9 7 2	0	0
2	C	1	Total O P 9 7 2	0	0
2	D	1	Total O P 9 7 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0
3	B	3	Total Mg 3 3	0	0
3	C	3	Total Mg 3 3	0	0
3	D	3	Total Mg 3 3	0	0

- Molecule 4 is (1S,5S,8S,9aR)-1,9a-dimethyl-8-(prop-1-en-2-yl)octahydro-2H-quinolizinium (three-letter code: JF1) (formula: C₁₄H₂₆N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 15 14 1	0	0
4	B	1	Total C N 15 14 1	0	0
4	C	1	Total C N 15 14 1	0	0
4	D	1	Total C N 15 14 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	379	Total O 379 379	0	0
6	B	295	Total O 295 295	0	0
6	C	214	Total O 214 214	0	0
6	D	111	Total O 111 111	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: Aristolochene synthase

Chain A:  91% . . .




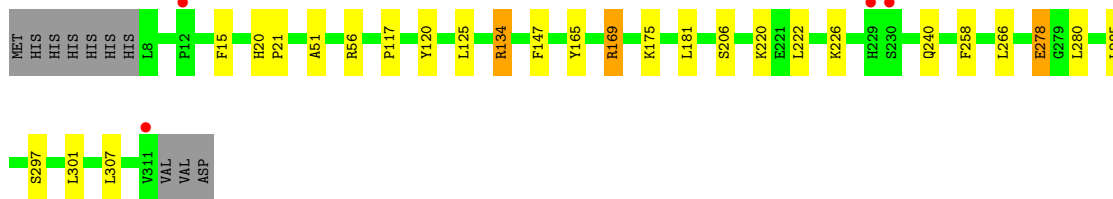
- Molecule 1: Aristolochene synthase

Chain B:  91% 5% . . .




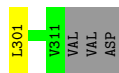
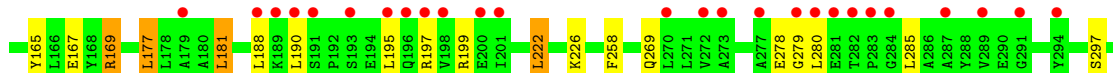
- Molecule 1: Aristolochene synthase

Chain C:  88% 8% . . .



- Molecule 1: Aristolochene synthase

Chain D:  87% 14% 9% . . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.85Å 123.85Å 202.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.38 – 2.04 47.38 – 2.04	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.38-2.04) 100.0 (47.38-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.03Å)	Xtrriage
Refinement program	PHENIX dev_1803	Depositor
R, R_{free}	0.203 , 0.235 0.203 , 0.237	Depositor DCC
R_{free} test set	2006 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10968	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: JF1, GOL, POP, MG

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	0.23	0/2525	0.39	0/3416
1	B	0.23	0/2514	0.38	0/3402
1	C	0.22	0/2525	0.37	0/3416
1	D	0.21	0/2514	0.36	0/3402
All	All	0.22	0/10078	0.37	0/13636

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	2467	0	2444	9	0
1	B	2456	0	2433	9	0
1	C	2464	0	2446	11	0
1	D	2456	0	2434	12	0
2	A	9	0	0	1	0
2	B	9	0	0	1	0
2	C	9	0	0	1	0
2	D	9	0	0	1	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	15	0	26	0	0
4	B	15	0	26	0	0
4	C	15	0	26	0	0
4	D	15	0	26	0	0
5	A	6	0	8	0	0
5	C	12	0	16	0	0
6	A	379	0	0	4	0
6	B	295	0	0	2	0
6	C	214	0	0	3	0
6	D	111	0	0	1	0
All	All	10968	0	9885	41	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 (41) 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:165:TYR:CZ	1:A:169:ARG:HG3	2.23	0.74
1:C:165:TYR:CZ	1:C:169:ARG:HG3	2.25	0.70
1:B:165:TYR:CZ	1:B:169:ARG:HG3	2.29	0.66
1:D:165:TYR:CZ	1:D:169:ARG:HG3	2.31	0.65
1:B:107:ARG:NH1	6:B:502:HOH:O	2.27	0.65
1:C:134:ARG:NH1	6:C:505:HOH:O	2.31	0.64
1:D:35:LEU:O	1:D:46:ARG:NH2	2.31	0.64
1:A:56:ARG:NH1	6:A:502:HOH:O	2.27	0.64
1:B:197:ARG:HD3	1:B:280:LEU:HB3	1.81	0.62
1:D:149:ARG:NH1	6:D:1004:HOH:O	2.36	0.59
1:B:222:LEU:HD22	1:B:226:LYS:HE3	1.86	0.57
1:C:51:ALA:HB1	1:C:307:LEU:HD12	1.87	0.56
1:C:169:ARG:HH22	2:C:401:POP:P1	2.30	0.55
1:D:66:LEU:HD12	1:D:69:ARG:HH12	1.72	0.54
1:B:169:ARG:NH2	2:B:401:POP:O2	2.32	0.54
1:C:15:PHE:HB3	1:C:297:SER:HB3	1.91	0.53
1:D:278:GLU:O	1:D:280:LEU:N	2.42	0.53
1:C:56:ARG:NH1	6:C:507:HOH:O	2.35	0.53
1:C:278:GLU:HB2	1:C:280:LEU:HG	1.91	0.53
1:D:169:ARG:HH22	2:D:401:POP:P1	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NH1	6:A:512:HOH:O	2.42	0.51
1:D:117:PRO:HA	1:D:120:TYR:CE2	2.47	0.50
1:D:15:PHE:HB3	1:D:297:SER:HB3	1.94	0.49
1:A:169:ARG:NH2	2:A:401:POP:O1	2.34	0.48
1:D:222:LEU:HD22	1:D:226:LYS:HE3	1.94	0.48
1:D:177:LEU:O	1:D:181:LEU:HB2	2.16	0.46
1:B:117:PRO:HA	1:B:120:TYR:CE2	2.51	0.45
1:B:196:GLN:O	1:B:199:ARG:HG2	2.17	0.45
1:D:195:LEU:O	1:D:199:ARG:NE	2.51	0.44
1:C:117:PRO:HA	1:C:120:TYR:CE2	2.52	0.44
1:B:285:LEU:HD12	1:B:285:LEU:HA	1.79	0.44
1:A:51:ALA:HB1	1:A:307:LEU:HD23	2.00	0.43
1:A:285:LEU:HD12	1:A:285:LEU:HA	1.92	0.43
1:C:20:HIS:HA	1:C:21:PRO:HD3	1.90	0.42
1:B:69:ARG:HD2	6:B:629:HOH:O	2.19	0.42
1:D:14:THR:OG1	1:D:269:GLN:NE2	2.42	0.42
1:A:69:ARG:HD2	6:A:633:HOH:O	2.19	0.42
1:A:43:GLU:HG3	1:A:47:LYS:HD3	2.02	0.41
1:C:175:LYS:HG2	1:C:206:SER:HB2	2.03	0.40
1:C:220:LYS:NZ	6:C:522:HOH:O	2.48	0.40
1:A:158:ARG:NH1	6:A:528:HOH:O	2.53	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	304/314 (97%)	301 (99%)	3 (1%)	0	100	100
1	B	303/314 (96%)	298 (98%)	5 (2%)	0	100	100
1	C	304/314 (97%)	298 (98%)	6 (2%)	0	100	100
1	D	303/314 (96%)	289 (95%)	12 (4%)	2 (1%)	22	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1214/1256 (97%)	1186 (98%)	26 (2%)	2 (0%)	47 39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	279	GLY
1	D	133	ASP

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	267/275 (97%)	256 (96%)	11 (4%)	30 23
1	B	266/275 (97%)	257 (97%)	9 (3%)	37 30
1	C	267/275 (97%)	254 (95%)	13 (5%)	25 17
1	D	266/275 (97%)	252 (95%)	14 (5%)	22 14
All	All	1066/1100 (97%)	1019 (96%)	47 (4%)	28 21

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	125	LEU
1	A	134	ARG
1	A	169	ARG
1	A	209	LEU
1	A	222	LEU
1	A	240	GLN
1	A	258	PHE
1	A	285	LEU
1	A	307	LEU
1	A	311	VAL
1	B	134	ARG
1	B	169	ARG

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Mol	Chain	Res	Type
1	B	177	LEU
1	B	181	LEU
1	B	222	LEU
1	B	247	ASP
1	B	258	PHE
1	B	285	LEU
1	B	301	LEU
1	C	125	LEU
1	C	134	ARG
1	C	147	PHE
1	C	169	ARG
1	C	181	LEU
1	C	222	LEU
1	C	226	LYS
1	C	240	GLN
1	C	258	PHE
1	C	266	LEU
1	C	278	GLU
1	C	285	LEU
1	C	301	LEU
1	D	62	PHE
1	D	69	ARG
1	D	147	PHE
1	D	167	GLU
1	D	169	ARG
1	D	177	LEU
1	D	181	LEU
1	D	188	LEU
1	D	190	LEU
1	D	197	ARG
1	D	222	LEU
1	D	258	PHE
1	D	285	LEU
1	D	301	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 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
5	GOL	C	407	-	5,5,5	0.50	0	5,5,5	0.62	0
2	POP	A	401	3	6,8,8	0.79	0	13,13,13	1.13	1 (7%)
5	GOL	A	406	-	5,5,5	0.37	0	5,5,5	0.27	0
2	POP	D	401	3	6,8,8	0.76	0	13,13,13	1.09	1 (7%)
4	JF1	A	405	-	14,16,16	0.63	0	20,24,24	1.13	0
4	JF1	C	405	-	14,16,16	0.60	0	20,24,24	1.10	0
2	POP	C	401	3	6,8,8	0.75	0	13,13,13	1.30	1 (7%)
4	JF1	D	405	-	14,16,16	0.61	0	20,24,24	1.13	0
2	POP	B	401	3	6,8,8	0.76	0	13,13,13	1.26	1 (7%)
5	GOL	C	406	-	5,5,5	0.39	0	5,5,5	0.21	0
4	JF1	B	405	-	14,16,16	0.60	0	20,24,24	1.12	0

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
5	GOL	C	407	-	-	0/4/4/4	-
2	POP	A	401	3	-	0/6/6/6	-
5	GOL	A	406	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POP	D	401	3	-	5/6/6/6	-
4	JF1	A	405	-	-	0/4/32/32	0/2/2/2
4	JF1	C	405	-	-	0/4/32/32	0/2/2/2
2	POP	C	401	3	-	2/6/6/6	-
4	JF1	D	405	-	-	0/4/32/32	0/2/2/2
2	POP	B	401	3	-	0/6/6/6	-
5	GOL	C	406	-	-	1/4/4/4	-
4	JF1	B	405	-	-	0/4/32/32	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	POP	P2-O-P1	-3.06	122.33	132.83
2	A	401	POP	P2-O-P1	-3.01	122.49	132.83
2	C	401	POP	P2-O-P1	-2.82	123.17	132.83
2	D	401	POP	O3-P1-O	2.18	111.96	104.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	POP	P1-O-P2-O4
2	C	401	POP	P1-O-P2-O6
2	D	401	POP	P2-O-P1-O2
2	D	401	POP	P2-O-P1-O3
2	C	401	POP	P1-O-P2-O5
2	D	401	POP	P1-O-P2-O5
2	D	401	POP	P1-O-P2-O6
5	C	406	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	POP	1	0
2	D	401	POP	1	0
2	C	401	POP	1	0
2	B	401	POP	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	304/314 (96%)	-0.55	0 100 100	21, 29, 43, 65	0
1	B	304/314 (96%)	-0.56	3 (0%) 82 84	22, 32, 49, 65	0
1	C	304/314 (96%)	-0.33	4 (1%) 77 79	28, 42, 63, 87	0
1	D	304/314 (96%)	0.66	45 (14%) 2 1	36, 58, 90, 107	0
All	All	1216/1256 (96%)	-0.20	52 (4%) 35 38	21, 38, 75, 107	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	LEU	6.6
1	C	230	SER	6.2
1	D	195	LEU	5.4
1	D	198	VAL	5.3
1	D	18	LEU	5.1
1	C	311	VAL	4.9
1	D	279	GLY	4.7
1	D	188	LEU	4.7
1	D	197	ARG	4.0
1	D	193	SER	3.9
1	D	190	LEU	3.8
1	D	277	ALA	3.8
1	D	23	VAL	3.5
1	D	189	LYS	3.3
1	D	284	GLY	3.2
1	D	111	LEU	3.1
1	D	283	PRO	3.0
1	D	281	GLU	3.0
1	D	70	ILE	2.9
1	D	272	VAL	2.9
1	D	108	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	289	VAL	2.7
1	D	201	ILE	2.6
1	D	25	GLU	2.4
1	D	19	CYS	2.4
1	D	287	ALA	2.4
1	D	282	THR	2.4
1	D	56	ARG	2.3
1	D	191	SER	2.3
1	B	279	GLY	2.3
1	D	294	TYR	2.3
1	C	229	HIS	2.3
1	B	280	LEU	2.3
1	D	66	LEU	2.3
1	D	200	GLU	2.3
1	D	145	PHE	2.2
1	D	291	GLY	2.2
1	D	129	MET	2.2
1	D	73	ALA	2.2
1	D	273	ALA	2.2
1	D	123	TYR	2.2
1	D	196	GLN	2.1
1	D	270	LEU	2.1
1	D	16	GLN	2.1
1	D	179	ALA	2.1
1	B	199	ARG	2.1
1	D	22	LEU	2.1
1	D	14	THR	2.0
1	D	139	GLU	2.0
1	D	21	PRO	2.0
1	C	12	PRO	2.0
1	D	126	TRP	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, 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
5	GOL	C	406	6/6	0.84	0.12	32,40,48,49	0
3	MG	D	404	1/1	0.86	0.17	40,40,40,40	0
5	GOL	C	407	6/6	0.88	0.16	41,54,60,66	0
3	MG	D	402	1/1	0.92	0.15	38,38,38,38	0
3	MG	C	402	1/1	0.93	0.07	40,40,40,40	0
4	JF1	A	405	15/15	0.94	0.13	24,33,39,40	0
3	MG	D	403	1/1	0.94	0.08	36,36,36,36	0
3	MG	C	403	1/1	0.94	0.04	32,32,32,32	0
4	JF1	B	405	15/15	0.95	0.12	25,33,39,41	0
4	JF1	D	405	15/15	0.95	0.14	40,57,61,68	0
5	GOL	A	406	6/6	0.95	0.07	32,38,41,43	0
3	MG	B	404	1/1	0.95	0.13	28,28,28,28	0
3	MG	C	404	1/1	0.95	0.14	38,38,38,38	0
3	MG	B	403	1/1	0.96	0.10	27,27,27,27	0
4	JF1	C	405	15/15	0.96	0.12	35,39,46,55	0
2	POP	D	401	9/9	0.97	0.11	29,43,47,55	0
3	MG	B	402	1/1	0.98	0.14	29,29,29,29	0
2	POP	C	401	9/9	0.98	0.10	30,36,44,47	0
3	MG	A	402	1/1	0.98	0.13	24,24,24,24	0
3	MG	A	403	1/1	0.98	0.13	23,23,23,23	0
2	POP	B	401	9/9	0.99	0.10	24,25,29,29	0
3	MG	A	404	1/1	0.99	0.11	24,24,24,24	0
2	POP	A	401	9/9	0.99	0.12	20,21,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.