



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2016 – 01:50 PM EDT

PDB ID : 5IMN
Title : Crystal structure of N299A/S303A *Aspergillus terreus* aristolochene synthase complexed with (1S,8S,9aR)-1,9a-dimethyl-8-(prop-1-en-2-yl)decahydroquinolin-5-ium
Authors : Chen, M.; Christianson, D.W.
Deposited on : 2016-03-06
Resolution : 2.53 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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) : rb-20027674

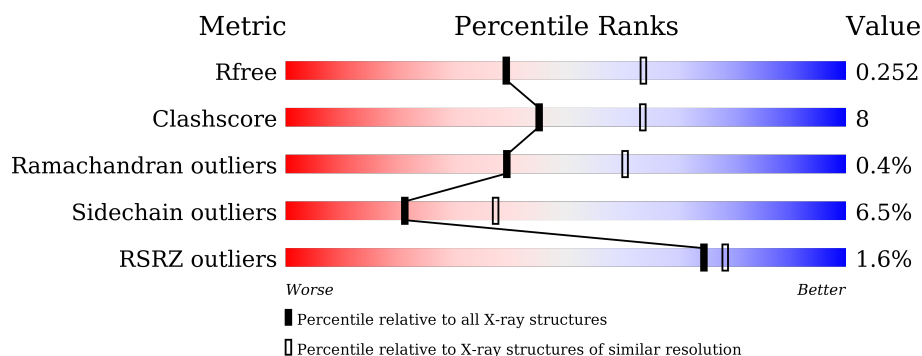
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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. 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	<div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	B	314	<div> <div>78%</div> <div>18%</div> <div>• •</div> </div>
1	C	314	<div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	D	314	<div> <div>5%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POP	B	401	-	-	X	-
4	GOL	A	405	-	-	-	X
5	JF1	A	406	-	-	-	X
5	JF1	B	405	-	-	-	X
5	JF1	D	405	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10238 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
1	A	304	Total	C	N	O	S	0	1	0
			2455	1569	414	456	16			
1	B	304	Total	C	N	O	S	0	2	0
			2463	1574	417	456	16			
1	C	304	Total	C	N	O	S	0	1	0
			2455	1569	414	456	16			
1	D	304	Total	C	N	O	S	0	2	0
			2463	1574	417	456	16			

There are 36 discrepancies between the modelled and reference sequences:

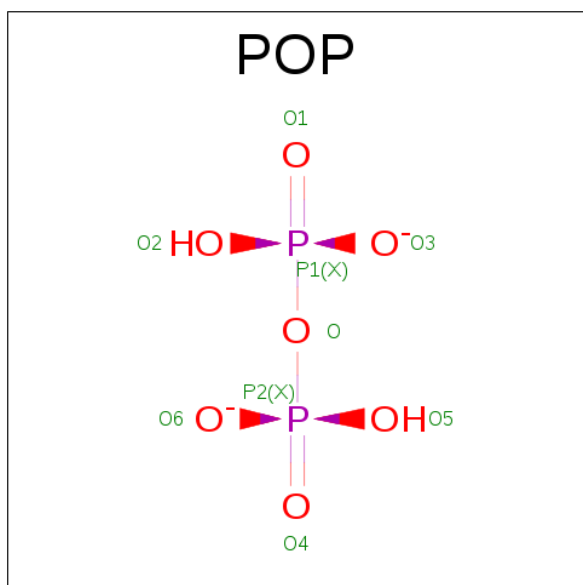
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9UR08
A	2	HIS	-	expression tag	UNP Q9UR08
A	3	HIS	-	expression tag	UNP Q9UR08
A	4	HIS	-	expression tag	UNP Q9UR08
A	5	HIS	-	expression tag	UNP Q9UR08
A	6	HIS	-	expression tag	UNP Q9UR08
A	7	HIS	-	expression tag	UNP Q9UR08
A	299	ALA	ASN	engineered mutation	UNP Q9UR08
A	303	ALA	SER	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
B	303	ALA	SER	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	HIS	-	expression tag	UNP Q9UR08
C	5	HIS	-	expression tag	UNP Q9UR08
C	6	HIS	-	expression tag	UNP Q9UR08
C	7	HIS	-	expression tag	UNP Q9UR08
C	299	ALA	ASN	engineered mutation	UNP Q9UR08
C	303	ALA	SER	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
D	303	ALA	SER	engineered mutation	UNP Q9UR08

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

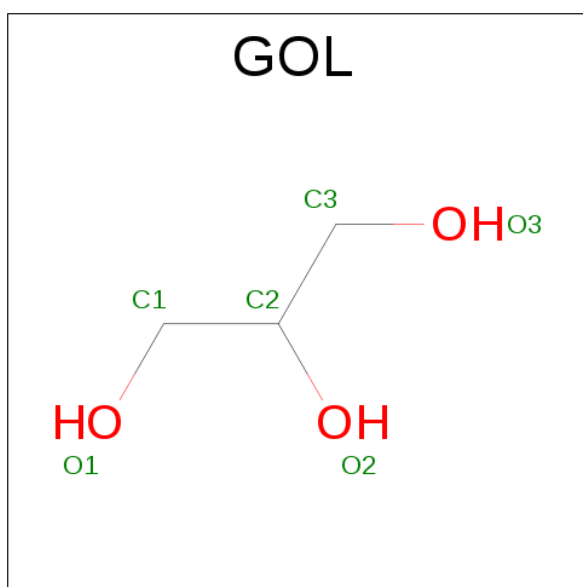


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 9 7 2	0	0
2	B	1	Total O P 9 7 2	0	0
2	C	1	Total O P 9 7 2	0	0
2	D	1	Total O P 9 7 2	0	0

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

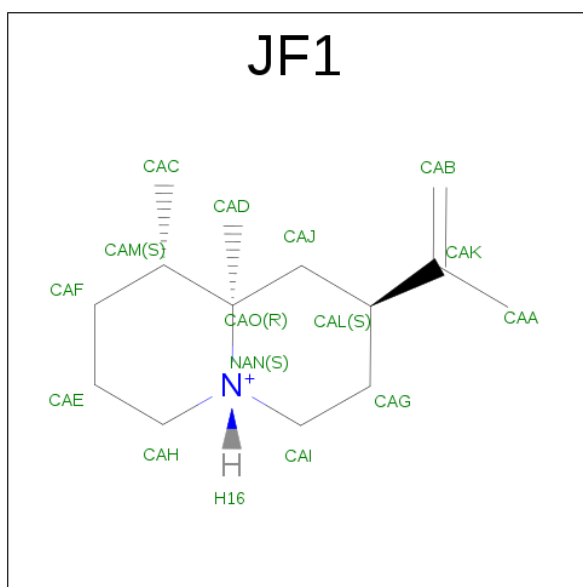
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Mg 3	0	0
3	A	3	Total 3	Mg 3	0	0
3	D	3	Total 3	Mg 3	0	0
3	C	3	Total 3	Mg 3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 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
5	A	1	Total	C	N	0	0
			15	14	1		
5	B	1	Total	C	N	0	0
			15	14	1		
5	C	1	Total	C	N	0	0
			15	14	1		
5	D	1	Total	C	N	0	0
			15	14	1		

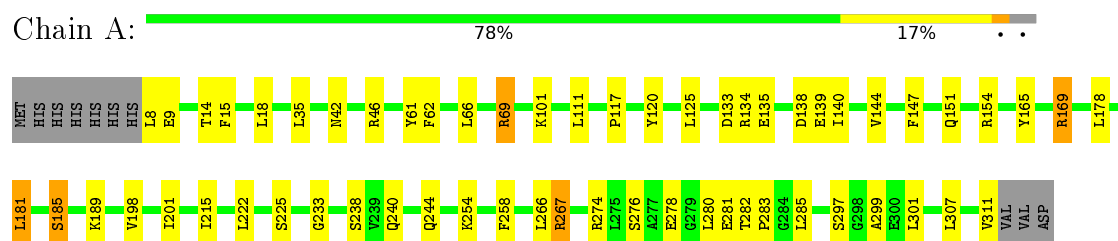
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	87	Total	O	0	0
			87	87		
6	C	43	Total	O	0	0
			43	43		
6	D	35	Total	O	0	0
			35	35		

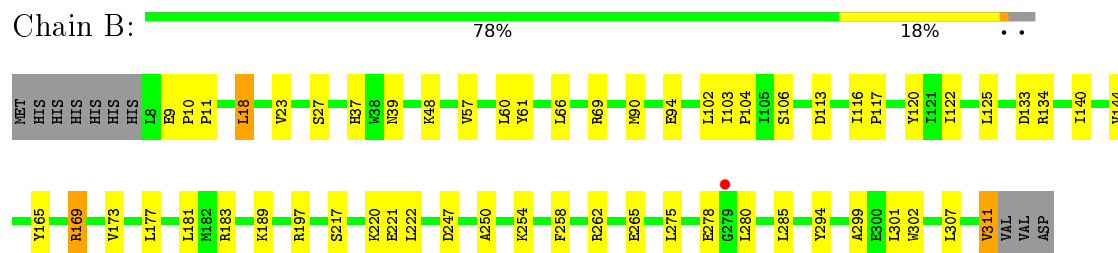
3 Residue-property plots

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.

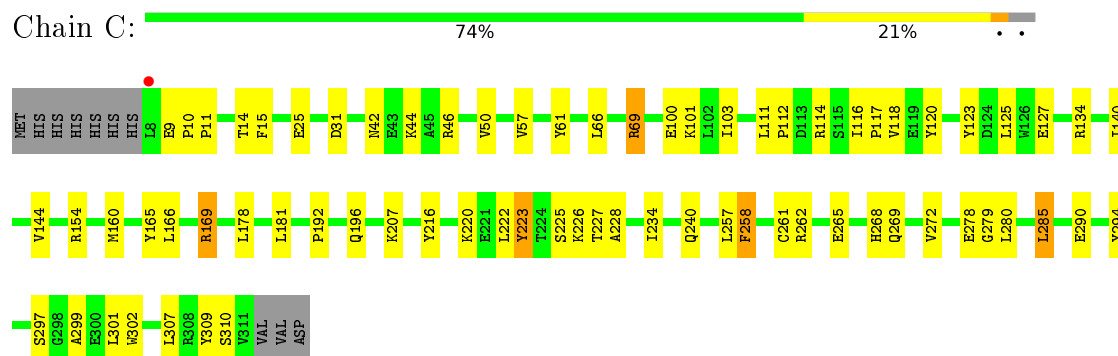
• Molecule 1: Aristolochene synthase



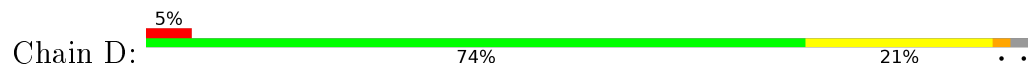
• Molecule 1: Aristolochene synthase

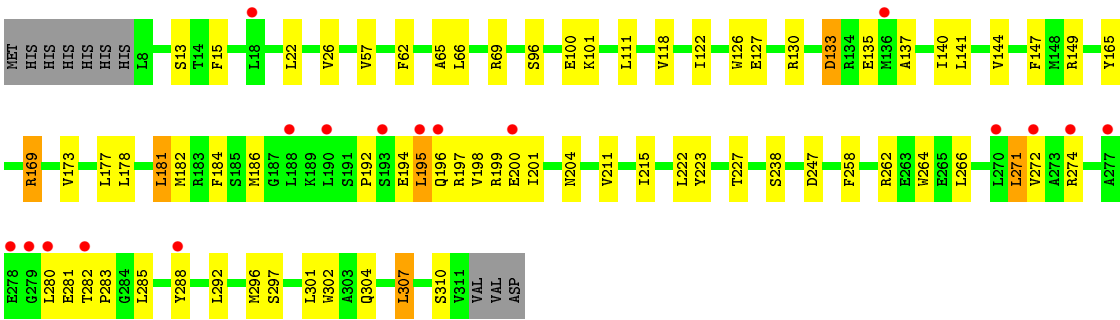


• Molecule 1: Aristolochene synthase



• Molecule 1: Aristolochene synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.30Å 124.30Å 202.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.53 – 2.53 47.53 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.53-2.53) 93.5 (47.53-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.195 , 0.254 0.189 , 0.252	Depositor DCC
R_{free} test set	1861 reflections (3.25%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10238	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, 0.375 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: GOL, MG, JF1, POP

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	0.47	0/2513	0.58	0/3401
1	B	0.46	0/2524	0.58	0/3415
1	C	0.41	0/2513	0.56	0/3401
1	D	0.40	0/2524	0.53	0/3415
All	All	0.43	0/10074	0.56	0/13632

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	2455	0	2433	31	0
1	B	2463	0	2447	32	0
1	C	2455	0	2434	43	0
1	D	2463	0	2447	42	0
2	A	9	0	0	2	0
2	B	9	0	0	4	0
2	C	9	0	0	2	0
2	D	9	0	0	2	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	6	0	8	0	0
5	A	15	0	26	1	0
5	B	15	0	26	3	0
5	C	15	0	26	1	0
5	D	15	0	26	4	0
6	A	123	0	0	5	0
6	B	87	0	0	2	0
6	C	43	0	0	2	0
6	D	35	0	0	2	0
All	All	10238	0	9873	155	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 8.

All (155) 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:D:194:GLU:HB3	1:D:285:LEU:HD11	1.60	0.83
1:C:169:ARG:NH2	2:C:401:POP:O1	2.14	0.81
1:C:278:GLU:HG2	1:C:280:LEU:HG	1.68	0.75
1:D:69:ARG:NH2	1:D:133:ASP:OD2	2.22	0.73
1:C:114:ARG:NH1	6:C:501:HOH:O	2.20	0.72
1:C:278:GLU:OE2	1:C:278:GLU:N	2.22	0.71
1:C:165:TYR:CZ	1:C:169:ARG:HG3	2.26	0.71
1:C:66:LEU:HD12	1:C:69:ARG:HD3	1.76	0.67
1:D:165:TYR:CZ	1:D:169:ARG:HG3	2.31	0.66
1:C:278:GLU:O	1:C:280:LEU:N	2.24	0.66
1:B:165:TYR:CZ	1:B:169:ARG:HG3	2.32	0.65
1:A:165:TYR:CZ	1:A:169:ARG:HG3	2.33	0.63
1:D:65:ALA:HA	1:D:186:MET:HG2	1.82	0.60
1:D:140:ILE:HD13	1:D:181:LEU:HD23	1.84	0.60
1:A:215:ILE:HG23	1:A:254:LYS:HG2	1.84	0.60
1:D:100:GLU:OE1	1:D:149:ARG:NH2	2.35	0.59
2:D:401:POP:O2	6:D:501:HOH:O	2.17	0.59
1:A:154:ARG:NH2	6:A:503:HOH:O	2.37	0.58
1:A:278:GLU:HB3	1:A:280:LEU:HG	1.86	0.58
1:A:178:LEU:HD11	5:A:406:JF1:H22	1.85	0.57
1:D:66:LEU:HD12	1:D:69:ARG:HD2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG12	1:A:201:ILE:HD12	1.87	0.56
1:A:240:GLN:OE1	1:A:244:GLN:NE2	2.39	0.56
1:D:118:VAL:O	1:D:122:ILE:HG12	2.06	0.56
1:C:46:ARG:O	1:C:50:VAL:HG23	2.06	0.56
1:B:117:PRO:HA	1:B:120:TYR:CE2	2.41	0.55
1:D:196:GLN:HG2	1:D:199:ARG:CZ	2.36	0.55
1:B:169:ARG:HH22	2:B:401:POP:P1	2.29	0.55
1:D:15:PHE:HB3	1:D:297:SER:HB3	1.90	0.54
1:B:66:LEU:HD12	1:B:69:ARG:HD3	1.90	0.54
1:C:42:ASN:OD1	1:C:44:LYS:HB3	2.08	0.54
1:B:197:ARG:HD3	1:B:280:LEU:HB3	1.88	0.53
1:C:223:TYR:HE2	1:C:227:THR:HG21	1.74	0.53
1:B:102:LEU:HD22	1:B:122:ILE:HD12	1.91	0.53
1:D:192:PRO:HA	1:D:195:LEU:HB2	1.91	0.53
1:D:223:TYR:CZ	1:D:227:THR:HG21	2.44	0.53
1:B:113:ASP:HB3	1:B:116:ILE:HD12	1.90	0.52
1:D:13:SER:HB2	1:D:262:ARG:CZ	2.39	0.52
1:A:267:ARG:NH1	6:A:506:HOH:O	2.39	0.52
1:B:140:ILE:O	1:B:144:VAL:HG23	2.10	0.52
1:B:217:SER:O	1:B:221:GLU:HG3	2.10	0.52
1:C:100:GLU:HA	1:C:103:ILE:HD12	1.91	0.52
1:B:220:LYS:NZ	2:B:401:POP:O5	2.39	0.52
1:D:144:VAL:HG22	1:D:177:LEU:HD22	1.91	0.52
1:A:169:ARG:NH2	2:A:401:POP:O1	2.40	0.51
1:C:66:LEU:HB2	1:C:69:ARG:HG2	1.93	0.51
1:B:90:MET:HB3	1:B:94:GLU:HB2	1.91	0.51
1:A:35:LEU:O	1:A:46:ARG:NH2	2.44	0.50
1:C:117:PRO:HA	1:C:120:TYR:CE2	2.46	0.50
1:C:160:MET:HE3	1:C:165:TYR:HD2	1.76	0.50
1:C:166:LEU:HD13	1:C:207:LYS:HG2	1.92	0.50
1:D:198:VAL:O	1:D:201:ILE:HG22	2.11	0.50
1:D:307:LEU:HA	1:D:310:SER:OG	2.10	0.50
1:C:192:PRO:O	1:C:196:GLN:HG2	2.11	0.50
1:C:220:LYS:NZ	2:C:401:POP:O5	2.45	0.50
1:C:178:LEU:HD11	5:C:405:JF1:H22	1.93	0.50
1:A:165:TYR:CE2	1:A:169:ARG:HG3	2.46	0.50
1:A:165:TYR:CE1	1:A:238:SER:HB3	2.47	0.49
1:B:250:ALA:O	1:B:254:LYS:HG3	2.13	0.49
1:B:48:LYS:NZ	1:B:311:VAL:HG11	2.28	0.49
1:C:290:GLU:HG2	1:C:294:TYR:CE1	2.48	0.49
1:A:135:GLU:O	1:A:139:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:TYR:HE2	1:C:299:ALA:HB2	1.78	0.48
1:B:169:ARG:NH2	2:B:401:POP:O2	2.45	0.48
1:D:62:PHE:HD2	1:D:182:MET:HG3	1.79	0.48
1:A:15:PHE:HB3	1:A:297:SER:HB3	1.95	0.48
1:C:42:ASN:O	1:C:46:ARG:HG3	2.14	0.47
1:C:57:VAL:HB	1:C:302:TRP:CD1	2.49	0.47
1:B:61:TYR:HE1	1:B:299:ALA:HB2	1.78	0.47
1:D:178:LEU:HD11	5:D:405:JF1:H22	1.96	0.47
1:C:25:GLU:N	1:C:25:GLU:OE1	2.40	0.47
1:B:183:ARG:NH1	6:B:501:HOH:O	2.24	0.47
1:C:216:TYR:O	1:C:309:TYR:HB3	2.15	0.47
1:D:22:LEU:O	1:D:26:VAL:HG23	2.14	0.47
1:A:181:LEU:O	1:A:185:SER:OG	2.32	0.47
1:A:42:ASN:O	1:A:46:ARG:HG3	2.15	0.47
1:B:69:ARG:NH2	1:B:133:ASP:OD2	2.44	0.47
1:C:165:TYR:OH	1:C:169:ARG:HG3	2.15	0.46
1:D:165:TYR:CE1	1:D:238:SER:HB3	2.50	0.46
1:A:165:TYR:OH	1:A:169:ARG:HD2	2.16	0.46
1:C:265:GLU:O	1:C:269:GLN:HG3	2.16	0.46
1:D:140:ILE:HD11	1:D:184:PHE:HB2	1.97	0.46
1:A:69:ARG:NH2	1:A:133:ASP:OD2	2.49	0.46
1:A:117:PRO:HA	1:A:120:TYR:CE2	2.51	0.46
1:A:61:TYR:HE1	1:A:299:ALA:HB2	1.80	0.45
1:B:39:ASN:HB2	6:B:568:HOH:O	2.16	0.45
1:C:261:CYS:O	1:C:265:GLU:HG3	2.16	0.45
1:D:127:GLU:CD	1:D:130:ARG:HH11	2.18	0.45
1:D:96:SER:O	1:D:100:GLU:HB2	2.16	0.45
1:C:257:LEU:HD23	1:C:257:LEU:HA	1.84	0.45
1:D:137:ALA:HB2	1:D:184:PHE:HE1	1.81	0.45
1:D:204:ASN:ND2	1:D:264:TRP:O	2.44	0.45
1:D:283:PRO:HD2	6:D:533:HOH:O	2.17	0.45
1:C:112:PRO:HD3	1:C:123:TYR:CD1	2.51	0.44
1:B:197:ARG:HG2	1:B:275:LEU:HD11	1.98	0.44
1:A:282:THR:HB	6:A:614:HOH:O	2.17	0.44
1:C:9:GLU:HA	1:C:10:PRO:HD3	1.69	0.44
1:A:8:LEU:HD12	1:A:9:GLU:H	1.82	0.44
1:C:262:ARG:NH1	1:C:265:GLU:OE2	2.45	0.44
1:D:141:LEU:HA	1:D:141:LEU:HD23	1.84	0.44
1:A:62:PHE:CE1	1:A:181:LEU:HD13	2.52	0.43
1:C:15:PHE:HB3	1:C:297:SER:HB3	2.00	0.43
2:B:401:POP:O2	5:B:405:JF1:H17	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:VAL:HB	1:D:302:TRP:CD2	2.52	0.43
1:B:165:TYR:OH	1:B:169:ARG:HD2	2.18	0.43
1:D:201:ILE:HD11	1:D:272:VAL:HG23	2.01	0.43
1:D:200:GLU:HG3	1:D:271:LEU:HD11	2.00	0.43
1:C:11:PRO:HD2	1:C:258:PHE:CD2	2.53	0.43
1:C:116:ILE:HG22	1:C:118:VAL:HG12	2.00	0.43
1:D:126:TRP:HB3	1:D:130:ARG:NH2	2.33	0.43
1:B:18:LEU:HD22	1:B:294:TYR:CE2	2.54	0.43
1:C:222:LEU:O	1:C:225:SER:OG	2.29	0.43
1:D:169:ARG:HH22	2:D:401:POP:P1	2.41	0.43
1:A:135:GLU:OE1	1:A:189:LYS:NZ	2.41	0.42
1:A:283:PRO:HD2	6:A:614:HOH:O	2.19	0.42
1:B:165:TYR:CE2	1:B:169:ARG:HG3	2.54	0.42
1:D:211:VAL:O	1:D:215:ILE:HG13	2.18	0.42
1:C:140:ILE:O	1:C:144:VAL:HG23	2.18	0.42
1:D:57:VAL:HB	1:D:302:TRP:CE2	2.55	0.42
5:D:405:JF1:H14	5:D:405:JF1:H3	1.64	0.42
1:C:307:LEU:HA	1:C:310:SER:HB3	2.00	0.42
1:B:23:VAL:O	1:B:27:SER:HB2	2.19	0.42
1:A:169:ARG:HH22	2:A:401:POP:P1	2.41	0.42
1:B:57:VAL:HB	1:B:302:TRP:CD1	2.54	0.42
1:C:268:HIS:O	1:C:272:VAL:HG23	2.20	0.42
1:D:15:PHE:HE2	1:D:296:MET:HE1	1.85	0.42
1:D:126:TRP:HB3	1:D:130:ARG:HH22	1.83	0.42
1:A:151:GLN:HG2	6:A:546:HOH:O	2.19	0.42
1:C:123:TYR:CE2	1:C:127:GLU:HG3	2.55	0.42
1:D:197:ARG:NH2	1:D:280:LEU:HD22	2.34	0.41
5:D:405:JF1:H22	5:D:405:JF1:H2	1.87	0.41
1:A:66:LEU:HD12	1:A:69:ARG:CD	2.49	0.41
1:D:197:ARG:HD2	1:D:280:LEU:HB3	2.02	0.41
1:A:140:ILE:O	1:A:144:VAL:HG23	2.21	0.41
1:B:37:HIS:O	1:B:117:PRO:HB3	2.20	0.41
1:B:278:GLU:C	1:B:280:LEU:H	2.24	0.41
1:B:9:GLU:HA	1:B:10:PRO:HD3	1.91	0.41
1:C:178:LEU:HD23	1:C:178:LEU:HA	1.80	0.41
1:C:285:LEU:HD12	1:C:285:LEU:HA	1.88	0.41
1:A:225:SER:HA	1:A:233:GLY:O	2.20	0.41
1:B:262:ARG:NH1	1:B:265:GLU:OE2	2.51	0.41
5:B:405:JF1:H14	5:B:405:JF1:H3	1.58	0.41
5:B:405:JF1:H21	5:B:405:JF1:H4	1.85	0.41
1:C:57:VAL:HB	1:C:302:TRP:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:LYS:HE3	1:D:101:LYS:HB2	1.72	0.41
5:D:405:JF1:H9	5:D:405:JF1:H2	1.87	0.41
1:D:140:ILE:HD11	1:D:184:PHE:CB	2.51	0.41
1:C:101:LYS:NZ	6:C:511:HOH:O	2.54	0.41
1:A:276:SER:HB2	1:A:281:GLU:OE2	2.21	0.40
1:B:103:ILE:HB	1:B:104:PRO:HD3	2.02	0.40
1:B:57:VAL:HB	1:B:302:TRP:CE2	2.56	0.40
1:D:196:GLN:HG2	1:D:199:ARG:NH2	2.36	0.40
1:B:10:PRO:HA	1:B:11:PRO:HD3	1.94	0.40
1:B:60:LEU:HA	1:B:60:LEU:HD23	1.94	0.40
1:D:288:TYR:HE2	1:D:292:LEU:HD11	1.87	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	303/314 (96%)	297 (98%)	6 (2%)	0	100	100
1	B	304/314 (97%)	299 (98%)	5 (2%)	0	100	100
1	C	303/314 (96%)	293 (97%)	8 (3%)	2 (1%)	26	45
1	D	304/314 (97%)	288 (95%)	13 (4%)	3 (1%)	19	33
All	All	1214/1256 (97%)	1177 (97%)	32 (3%)	5 (0%)	39	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	228	ALA
1	C	279	GLY
1	D	133	ASP
1	D	135	GLU

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Mol	Chain	Res	Type
1	D	281	GLU

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	265/274 (97%)	244 (92%)	21 (8%)	15	27
1	B	266/274 (97%)	250 (94%)	16 (6%)	24	41
1	C	265/274 (97%)	249 (94%)	16 (6%)	24	41
1	D	266/274 (97%)	250 (94%)	16 (6%)	24	41
All	All	1062/1096 (97%)	993 (94%)	69 (6%)	21	37

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	18	LEU
1	A	69	ARG
1	A	101	LYS
1	A	111	LEU
1	A	125	LEU
1	A	134	ARG
1	A	138	ASP
1	A	147	PHE
1	A	169	ARG
1	A	181	LEU
1	A	185	SER
1	A	222	LEU
1	A	258	PHE
1	A	266	LEU
1	A	267	ARG
1	A	274	ARG
1	A	285	LEU
1	A	301	LEU
1	A	307	LEU

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Mol	Chain	Res	Type
1	A	311	VAL
1	B	18	LEU
1	B	106	SER
1	B	125	LEU
1	B	134	ARG
1	B	169	ARG
1	B	173	VAL
1	B	177	LEU
1	B	181	LEU
1	B	189	LYS
1	B	222	LEU
1	B	247	ASP
1	B	258	PHE
1	B	285	LEU
1	B	301	LEU
1	B	307	LEU
1	B	311	VAL
1	C	14	THR
1	C	31	ASP
1	C	69	ARG
1	C	111	LEU
1	C	125	LEU
1	C	134	ARG
1	C	154	ARG
1	C	169	ARG
1	C	181	LEU
1	C	223	TYR
1	C	226	LYS
1	C	234	ILE
1	C	240	GLN
1	C	258	PHE
1	C	285	LEU
1	C	301	LEU
1	D	111	LEU
1	D	147	PHE
1	D	169	ARG
1	D	173	VAL
1	D	181	LEU
1	D	195	LEU
1	D	222	LEU
1	D	247	ASP
1	D	258	PHE

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Mol	Chain	Res	Type
1	D	266	LEU
1	D	271	LEU
1	D	274	ARG
1	D	282	THR
1	D	301	LEU
1	D	304	GLN
1	D	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	244	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 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
2	POP	A	401	3	8,8,8	0.70	0	13,13,13	1.38	1 (7%)
4	GOL	A	405	-	5,5,5	0.34	0	5,5,5	0.28	0
5	JF1	A	406	-	14,16,16	0.91	1 (7%)	20,24,24	1.87	4 (20%)
2	POP	B	401	3	8,8,8	0.59	0	13,13,13	1.21	2 (15%)
5	JF1	B	405	-	14,16,16	0.85	1 (7%)	20,24,24	2.16	6 (30%)
2	POP	C	401	3	8,8,8	0.51	0	13,13,13	1.50	3 (23%)
5	JF1	C	405	-	14,16,16	0.69	0	20,24,24	1.55	3 (15%)
2	POP	D	401	3	8,8,8	0.57	0	13,13,13	1.58	2 (15%)
5	JF1	D	405	-	14,16,16	0.92	1 (7%)	20,24,24	2.04	4 (20%)

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
2	POP	A	401	3	-	0/6/6/6	0/0/0/0
4	GOL	A	405	-	-	0/4/4/4	0/0/0/0
5	JF1	A	406	-	-	0/4/32/32	0/2/2/2
2	POP	B	401	3	-	0/6/6/6	0/0/0/0
5	JF1	B	405	-	-	0/4/32/32	0/2/2/2
2	POP	C	401	3	-	0/6/6/6	0/0/0/0
5	JF1	C	405	-	-	0/4/32/32	0/2/2/2
2	POP	D	401	3	-	0/6/6/6	0/0/0/0
5	JF1	D	405	-	-	0/4/32/32	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	405	JF1	CAO-CAM	-3.13	1.50	1.55
5	A	406	JF1	CAO-CAM	-2.90	1.51	1.55
5	B	405	JF1	CAO-CAM	-2.79	1.51	1.55

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	405	JF1	CAC-CAM-CAO	-5.26	107.33	114.10
5	B	405	JF1	CAC-CAM-CAO	-4.70	108.05	114.10
5	B	405	JF1	CAH-NAN-CAO	-4.62	107.95	113.07
5	D	405	JF1	CAH-NAN-CAO	-4.31	108.29	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	JF1	CAH-NAN-CAO	-4.09	108.54	113.07
5	A	406	JF1	CAC-CAM-CAO	-3.97	108.99	114.10
2	A	401	POP	P2-O-P1	-3.88	121.40	132.51
5	B	405	JF1	CAO-CAJ-CAL	-3.63	106.89	114.47
5	A	406	JF1	CAO-CAJ-CAL	-3.38	107.41	114.47
2	C	401	POP	P2-O-P1	-3.31	123.03	132.51
5	C	405	JF1	CAO-CAJ-CAL	-3.29	107.59	114.47
5	D	405	JF1	CAO-CAJ-CAL	-3.28	107.62	114.47
5	B	405	JF1	CAE-CAH-NAN	-3.04	105.07	111.48
5	C	405	JF1	CAH-NAN-CAO	-2.93	109.82	113.07
5	A	406	JF1	CAJ-CAL-CAG	-2.89	106.07	109.67
5	C	405	JF1	CAC-CAM-CAO	-2.48	110.90	114.10
2	B	401	POP	P2-O-P1	-2.36	125.74	132.51
5	B	405	JF1	CAJ-CAL-CAG	-2.29	106.82	109.67
2	D	401	POP	P2-O-P1	-2.25	126.06	132.51
5	D	405	JF1	CAE-CAH-NAN	-2.08	107.10	111.48
2	C	401	POP	O3-P1-O	2.13	113.33	106.48
2	C	401	POP	O5-P2-O	2.36	111.77	104.29
2	B	401	POP	O5-P2-O	2.38	111.83	104.29
5	B	405	JF1	CAF-CAM-CAO	2.78	114.32	111.67
2	D	401	POP	O2-P1-O	3.46	115.24	104.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	POP	2	0
5	A	406	JF1	1	0
2	B	401	POP	4	0
5	B	405	JF1	3	0
2	C	401	POP	2	0
5	C	405	JF1	1	0
2	D	401	POP	2	0
5	D	405	JF1	4	0

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	304/314 (96%)	-0.34	0 100 100	34, 45, 60, 88	0
1	B	304/314 (96%)	-0.34	1 (0%) 94 95	36, 50, 70, 94	0
1	C	304/314 (96%)	-0.22	1 (0%) 94 95	44, 61, 80, 105	0
1	D	304/314 (96%)	0.35	17 (5%) 28 32	47, 71, 102, 117	0
All	All	1216/1256 (96%)	-0.14	19 (1%) 74 78	34, 55, 87, 117	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	LEU	4.4
1	D	195	LEU	4.1
1	D	188	LEU	3.9
1	D	279	GLY	3.7
1	D	18	LEU	3.6
1	D	196	GLN	3.3
1	D	274	ARG	3.3
1	D	190	LEU	3.1
1	D	272	VAL	3.0
1	B	279	GLY	2.6
1	C	8	LEU	2.4
1	D	270	LEU	2.4
1	D	277	ALA	2.4
1	D	288	TYR	2.3
1	D	136	MET	2.3
1	D	193	SER	2.2
1	D	282	THR	2.1
1	D	278	GLU	2.1
1	D	200	GLU	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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	JF1	D	405	15/15	0.92	0.31	3.49	66,69,89,98	0
4	GOL	A	405	6/6	0.90	0.25	3.17	54,58,64,64	0
5	JF1	B	405	15/15	0.96	0.21	2.59	45,53,63,66	0
5	JF1	A	406	15/15	0.94	0.20	2.34	48,55,62,62	0
3	MG	B	404	1/1	0.98	0.16	1.82	43,43,43,43	0
3	MG	C	403	1/1	0.98	0.15	1.68	53,53,53,53	0
3	MG	D	403	1/1	0.97	0.18	1.17	51,51,51,51	0
3	MG	C	404	1/1	0.79	0.17	0.94	55,55,55,55	0
3	MG	B	403	1/1	0.96	0.15	0.55	45,45,45,45	0
2	POP	A	401	9/9	0.99	0.15	0.51	31,37,41,44	0
5	JF1	C	405	15/15	0.96	0.17	0.16	52,65,82,82	0
2	POP	B	401	9/9	0.99	0.13	-0.19	38,43,47,47	0
3	MG	D	404	1/1	0.91	0.15	-0.55	47,47,47,47	0
2	POP	D	401	9/9	0.98	0.14	-0.60	50,54,60,66	0
2	POP	C	401	9/9	0.99	0.12	-0.70	52,59,69,73	0
3	MG	A	402	1/1	0.98	0.15	-	41,41,41,41	0
3	MG	C	402	1/1	0.95	0.16	-	68,68,68,68	0
3	MG	A	403	1/1	0.98	0.16	-	39,39,39,39	0
3	MG	D	402	1/1	0.90	0.16	-	47,47,47,47	0
3	MG	A	404	1/1	0.95	0.17	-	38,38,38,38	0
3	MG	B	402	1/1	0.92	0.16	-	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.